Classification of gauge groups in terms of algebraic structure of first class constraints

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Properties of gauge transformations for singular Lagrangians are investigated to classify types of gauge groups. A general method of the classification is proposed based on properties of structure functions of the Poisson brackets (or the commutators) of first class constraints. A remarkable result is that the algebraic structure of the gauge group is essentially determined by the first class constraints of the final step of constraint series which are required successively from the stationarity conditions of the constraints. Owing to this consequence, the classification of gauge groups is made simple and transparent. The structure and property of the gauge group can be characterized in terms of the algebraic structure functions among the final step constraints and the number of the steps of the constraints series. The formulation proposed will give a clue to find new types of gauge groups.

I. INTRODUCTION

Gauge invariant systems will become more important in particle physics. The concept of gauge invariance will become one of fundamental principles of field theory. The general method to get a local gauge theory from a global symmetry theory was given by Yang-Mills[1] and Utiyama.[2] On the other hand, it will be significant to investigate gauge properties of singular Lagrangians.

Since the gauge transformations (GT) are the operations preserving an action invariant, they make a group. It would be interesting to consider the structure of the gauge groups and to classify their types in terms of their generators. Furthermore, it is expected that the result will give a clue to finding new types of gauge theories.

The generator G of GT leaving the action invariant can be expressed in terms of a linear combination of first class constraints (FCC) appearing in its dynamical system.[3,4] It is therefore obvious that the algebraic structure and the properties of the gauge group are determined by the structure functions (in general, functions of dynamical variables) of Poisson brackets (or commutators) of FCCs. But the algebraic structure of the gauge group is, in essential, determined by the FCCs of the final step of the constraint series which appear successively under stationarity conditions of the constraints. This fact is the most significant result in this paper.

In Sec. II, we will give a relation of the FCCs and the generator G. Next, general properties of G and the GT generated by G will be discussed. In Sec. III, characteristic properties and various relations for the algebraic structure functions of Poisson brackets among FCCs and Hamiltonian will be derived from the conditions required for G.

By using the results in Sec. II and III, it will be shown in Sec. IV that the algebraic structure of the gauge group is essentially given by the FCCs of the final step of the stationarity conditions. Owing to this important property, the classification of the gauge groups can be made simple and transparent. Section V will be devoted to discussion.

II. FIRST CLASS CONSTRAINTS AND GENERATOR OF GAUGE TRANSFORMATION

For the sake of simplicity, we consider a dynamical system with finite degrees of freedom, described by a Lagrangian $L(q,\dot{q})$ with dynamical variables q^i and $\dot{q}^i \equiv dq^i/dt$ $(i = 1 \sim N)$. If L is singular and the rank of the Hessian matrix

$$A_{ij} \equiv \frac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j} \tag{2.1}$$

is $N - A$, then there exist A primary constraints

$$\phi_\alpha^1(q,p) = 0 \quad (\alpha = 1 \sim A). \tag{2.2}$$

In this paper, we assume all constraints to be first class for simplicity. Systems including second class constraints (SCCs) can be treated in a similar way by using the formalism of Ref. 5, if the first class constraints and the Hamiltonian are in involution. But for illustration of the essential part of our analysis, we are sufficient with such systems.

In order for this system to have a consistent solution, ϕ_α^1 must be stationary. Following Dirac,[6] we introduce secondary constraints in phase space. The total Hamiltonian H_T is given by

$$H_T = H(q,p) + v^\alpha \phi_\alpha^1(q,p), \tag{2.3}$$

where a multiplier v^α is an arbitrary function of t and H is a canonical Hamiltonian. The summation convention is employed for dummy indices. In order to avoid complexity due to quantum anomaly and operator ordering, we consider classical theory here.

Let us define recurrently the series of constraints as

$$\phi_\alpha^{k+1} \equiv \{\phi_\alpha^k, H\} \quad (k = 1 \sim K - 1), \tag{2.4}$$

$$\{\phi_\alpha^K, H\} \equiv C_{\alpha k}^{\beta} \phi_\beta^k, \tag{2.5}$$

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with the stationarity conditions, where the symbol $\{\ ,\ \}$ denotes the Poisson bracket. These ϕ_α^k satisfy the involutive relation

$$\{\phi_\alpha^k,\phi_\beta^l\} = C_{\alpha\beta,m}^{kl\gamma}\phi_\gamma^m, \quad (\alpha,\beta,\gamma = 1\sim A,\quad k,l,m = 1\sim K). \tag{2.6}$$

We can express (2.4)–(2.6) as

$$\{\phi_A,H\} = C_A^B\phi_B,\quad \{\phi_A,\phi_B\} = C_{AB}^D\phi_D,$$

where $\phi_A = \{\phi_\alpha^1,\phi_\alpha^2,\ldots,\phi_\alpha^K\}$, but the definitions of (2.4)–(2.6) are convenient to the following argument. The maximal number K of ϕ_α^k will, in general, depend on α and should be written as K_α, but we omit the suffix α for the sake of simplicity.

Since the system has only FCCs, the set of ϕ_α^k defined in terms of H_T in place of H is equivalent to the set of ϕ_α^k of (2.4) and (2.5) (Ref. 4).

We observe in (2.4)–(2.6) that ϕ_α^k and H are in involution. Then, the generator G of the gauge transformation (GT) can be expressed as[3,4]

$$G = \epsilon_k^\alpha\phi_\alpha^k, \tag{2.7}$$

and should satisfy the conditions

$$\frac{\partial G}{\partial t} + \{G,H\} \equiv 0 \mod(\phi_\alpha^1), \tag{2.8}$$

$$\{G,\phi_\alpha^1\} \equiv 0 \mod(\phi_\beta^1). \tag{2.9}$$

Equations (2.8) and (2.9) are necessary and sufficient conditions for G to be the generator of GT leaving the action invariant. Equation (2.8) is nothing but the stationarity condition of G. It is crucial in this formulation that ϕ_α^1 identically vanishes in velocity phase space $(q^i,\dot q^i)$;

$$\phi_\alpha^1[q,p(q,\dot q)] \equiv 0. \tag{2.10}$$

Here, G thus defined contains A arbitrary infinitesimal functions $\epsilon^\alpha(t)$ $(\alpha = 1\sim A)$, which are gauge functions. The relation between $\epsilon^\alpha(t)$ and ϵ_k^α will be presented in Sec. III. The GT is given by

$$\delta q^i = \{q^i,G\},\qquad \delta\dot q^i = \frac{d}{dt}\{q^i,G\}, \tag{2.11}$$

and we obtain[4]

$$\delta L = \frac{d}{dt}\left(p_i\frac{\partial G}{\partial p_i} - G\right). \tag{2.12}$$

Inversely, if a variation of L is expressed as

$$\delta L = \frac{d}{dt}F(q,\dot q,\epsilon), \tag{2.13}$$

under the transformation

$$\delta q^i = \sum_{k=0}^{K-1}\overset{(k)}{\epsilon}{}^\alpha(t)f_{k\alpha}^i(q,\dot q), \tag{2.14}$$

with

$$\overset{(k)}{\epsilon}{}^\alpha(t) \equiv \frac{d^k}{dt^k}\epsilon^\alpha(t)\quad(\alpha = 1\sim A),$$

where $\epsilon^\alpha(t)$ is an arbitrary gauge function, we obtain

$$A_{ij}f_{K-1\alpha}^j \equiv 0\quad(\alpha = 1\sim A), \tag{2.15}$$

from identities derived from (2.13) and (2.14). Hence, this L is singular and the rank of A_{ij} is $N-A$. The kernel $f_{K-1\alpha}^i$ of A_{ij} is related to the primary constraint ϕ_α^1 by[3]

$$f_{K-1\alpha}^i = \frac{\partial\phi_\alpha^1}{\partial p_i}.$$

Further, it is shown that the generator yielding the GT of (2.14) is given by the above G. The characteristic property of the gauge group, therefore, can be ascribed to G.

Now let us denote the generators of GTs parametrized in terms of gauge functions $\epsilon_{(1)}^\alpha(t)$ and $\epsilon_{(2)}^\alpha(t)$ by $G(\epsilon_{(1)})$ and $G(\epsilon_{(2)})$, respectively. Then, the third generator

$$G(\epsilon_{(3)}) \equiv \{G(\epsilon_{(1)}),G(\epsilon_{(2)})\} \tag{2.16}$$

satisfies (2.8) and (2.9), owing to the Jacobi identity. Here, $G(\epsilon_{(3)})$ is also a linear combination of ϕ_α^k; that is,

$$G(\epsilon_{(3)}) = \epsilon_{(3)k}^\alpha\phi_\alpha^k, \tag{2.17}$$

since all ϕ_α^k are in involution. It may happen for $\epsilon_{(3)k}^\alpha$ to depend on ϕ_β^l. Even for this case, we call (2.17) a linear combination of ϕ_α^k. Hence, $G(\epsilon_{(3)})$ is also the generator of GT and comprises A-gauge functions $\epsilon_{(3)}^\alpha$, which are expressed in terms of $\epsilon_{(1)}^\alpha(t)$, $\epsilon_{(2)}^\alpha(t)$, $C_{\alpha k}^\beta$, and $C_{\alpha\beta,m}^{kl\gamma}$. Since the essential part of the gauge property is decided by (2.16), types of the gauge groups can be classified by functional forms of

$$\epsilon_{(3)}^\alpha = g^\alpha(\epsilon_{(1)}^\beta,\epsilon_{(2)}^\beta,C_{\beta k}^\gamma,C_{\beta\gamma,m}^{kl\delta}). \tag{2.18}$$

If $C_{\alpha\beta,m}^{kl\gamma}$ and/or $C_{\alpha k}^\beta$ depend on q and p (Refs. 7 and 8), $\epsilon_{(3)}^\alpha$ also is q and p dependent and the structure of the gauge groups will be complex. In the case of $g^\alpha \equiv 0$, $G(\epsilon_{(3)}) = 0$ and then the gauge group is inferred to be Abelian. If $G(\epsilon)$, however, involves powers of p higher than quadratic, we need careful consideration. For, the GT (2.11) in velocity phase space is not equivalent to the GT in phase space:

$$\delta q^i = \{q^i,G\} = \frac{\partial G}{\partial p_i},\quad \bar\delta p^i = \{p_i,G\} = -\frac{\partial G}{\partial q^i}, \tag{2.19}$$

if

$$\frac{\partial^2 G}{\partial p_i\,\partial p_j} \neq 0. \tag{2.20}$$

In fact, δp_i corresponding to (2.11) can be written as

$$\delta p_i(q,\dot q) = \frac{\partial p_i}{\partial q^j}\frac{\partial G}{\partial p_j} + A_{ij}\frac{d}{dt}\left(\frac{\partial G}{\partial p_j}\right), \tag{2.21}$$

and we obtain

$$\delta p_i - \bar\delta p_i = A_{ij}\frac{\partial^2 G}{\partial p_j\,\partial p_k}\left(\dot p_k - \frac{\partial L}{\partial q^k}\right). \tag{2.22}$$

Hence, both transformations accord under the equation of motion, namely, they are not equivalent for a transformation between two points off trajectories of motion. It means that though the equations of motion are invariant under both transformations, the action

$$S = \int L(q,\dot q)dt \tag{2.23}$$

is not necessarily invariant under the transformation (2.19).

Although the algebraic structure of GT in phase space is completely determined by (2.16) and (2.18), for the alge-

braic structure in velocity phase space, a further consideration is required. Since the generator of GT in velocity phase space is given, with (2.11), by

$$X=\delta q^i\frac{\partial}{\partial q^i}+\delta\dot{q}^i\frac{\partial}{\partial\dot{q}^i}, \tag{2.24}$$

we should examine the structure of the commutator $[X_1,X_2]$, where X_a denotes the generator associated with $G(\epsilon_{(a)})$. It should be noticed that if G contains higher powers of p, δq depends on $\dot{q}$ and $\delta\dot{q}$ on $\ddot{q}$, so that the commutators of X's do not close within themselves. Hence, we should employ the generator

$$X_E=\sum_{r=0}^{\infty}\left(\frac{d^r}{dt^r}\delta q^i\right)\frac{\partial}{\partial\overset{(r)}{q}{}^i} \tag{2.25}$$

in an infinite dimensional vector space, in order for the commutator algebra of X to close. This corresponds to the fact that higher derivatives $\overset{(r)}{q}$ successively appear in new transformed Lagrangians, through $d^r(\delta q)/dt^r$, by repeatedly applying GTs, since $L(q,\dot{q})$ turns out to be

$$L'(q,\dot{q},\ddot{q})=L(q,\dot{q})+\delta L(q,\dot{q},\ddot{q}), \tag{2.26}$$

where

$$\delta L=\frac{d}{dt}\left(p_i\frac{\partial G}{\partial p_i}-G\right)\equiv\frac{d}{dt}f,$$

under the GT generated by G.

If G is at most linear in p, f is a function of only q, and L' does not depend on $\ddot{q}$. In this case the commutators of X's given by (2.24) close within a $2N$-dimensional vector space. Denoting the GT generated by X_a in terms of δ_a $(a=1,2)$, we obtain

$$(\delta_2\delta_1-\delta_1\delta_2)L=\frac{d}{dt}(F+\overline{F}), \tag{2.27}$$

with

$$\begin{aligned}F&\equiv\left(p_i\frac{\partial}{\partial p_i}-1\right)\{G(\epsilon_{(1)}),G(\epsilon_{(2)})\}\\&=\left(p_i\frac{\partial}{\partial p_i}-1\right)G(\epsilon_{(3)}),\end{aligned} \tag{2.28}$$

$$\begin{aligned}\overline{F}&\equiv(\delta_2p_i-\bar{\delta}_2p_i)p_j\frac{\partial^2G(\epsilon_{(1)})}{\partial p_i\,\partial p_j}\\&\quad-(\delta_1p_i-\bar{\delta}_1p_i)p_j\frac{\partial^2G(\epsilon_{(2)})}{\partial p_i\,\partial p_j}.\end{aligned} \tag{2.29}$$

As seen from (2.28) and (2.29), $\overline{F}=0$ for $\partial^2G/\partial p_i\,\partial p_j=0$, and then the expressions of F and δL of (2.12) indicate the consistency between the transformations (2.11) and (2.19).

From the above, we observe that when $\overline{F}\neq0$, the gauge group is not necessarily Abelian, even if $G(\epsilon_{(3)})\equiv0$ in (2.16). If $[X_1,X_2]$ is not equivalent to $\{G(\epsilon_{(1)}),G(\epsilon_{(2)})\}$, the difference of $[X_1,X_2]$ and X_3 associated with $G(\epsilon_{(3)})$ seems at a glance to yield another independent GT. If so, there would exist a new GT which cannot be expressed in terms of $G(\epsilon)$ alone. In order to examine it, put

$$\Delta_{12}q^i\equiv[X_1,X_2]q^i \tag{2.30}$$

and

$$\delta_{12}q^i\equiv\frac{\partial}{\partial p_i}\{G(\epsilon_{(1)}),G(\epsilon_{(2)})\}. \tag{2.31}$$

We find

$$\delta'_{12}q^i\equiv\Delta_{12}q^i-\delta_{12}q^i=B^{ij}\left(\dot{p}_j-\frac{\partial L}{\partial q^j}\right), \tag{2.32}$$

where

$$B^{ij}=-B^{ji}=\frac{\partial^2G(\epsilon_{(1)})}{\partial p_i\,\partial p_k}A_{kl}\frac{\partial^2G(\epsilon_{(2)})}{\partial p_l\,\partial p_j}-(\epsilon_{(1)}\leftrightarrow\epsilon_{(2)}), \tag{2.33}$$

and the new GT $\delta'_{12}q^i$ produces

$$\delta'_{12}L=\frac{d}{dt}(p_i\delta'_{12}q^i)-\left(\dot{p}_i-\frac{\partial L}{\partial q^i}\right)\delta'_{12}q^i. \tag{2.34}$$

By substituting (2.32) into (2.34), the second term vanishes due to $B^{ij}=-B^{ji}$. For an arbitrary $B^{ij}=-B^{ji}$, the transformation of the form (2.32) always makes the action invariant. Then, $p_i\delta'_{12}q^i$ is a conserved quantity, but the Noether charge vanishes owing to $\delta'_{12}q^i=0$ under the equations of motion. Hence, $\delta'_{12}q^i$ is trivial transformation and we may suppose the GT to be essentially determined by $G(\epsilon)$ and their Poisson bracket.

Since GT always has the ambiguity by $B^{ij}(\dot{p}_j-\partial L/\partial q^j)$ that is trivial, we define the equivalent class of GTs with respect to the ambiguity. In what follows, we will consider the equivalent class of GTs (disregarding the ambiguity). We, however, should keep in mind that the algebraic property of GT cannot be completely determined only by the Poisson bracket of $G(\epsilon)$, if $\partial^2G/\partial p_i\,\partial p_j\neq0$.

III. RELATIONS AMONG STRUCTURE FUNCTIONS $C^{k\ell\gamma}_{\alpha\beta,m}$ AND $C^{\beta}_{\alpha k}$

In order to see the algebraic structure of the gauge group, we must obtain relations of ϵ^α_k to $C^\beta_{\alpha k}$, from the requirement that

$$G(\epsilon)=\epsilon^\alpha_k\phi^k_\alpha \tag{3.1}$$

should satisfy (2.8) and (2.9). With the help of (2.4) and (2.5), the substitution of (3.1) into (2.8) leads to

$$\dot{\epsilon}^\alpha_k+\epsilon^\alpha_{k-1}+C^\alpha_{\beta k}\epsilon^\beta_K=0\quad(2\leqslant k\leqslant K), \tag{3.2}$$

where

$$\dot{\epsilon}^\alpha_k\equiv\frac{\partial\epsilon^\alpha_k}{\partial t}+\{\epsilon^\alpha_k,H\}. \tag{3.3}$$

Equation (3.2) is the recurrence formula to decide $\epsilon^\alpha_k(k<K)$ by giving ϵ^α_K. Since ϵ^α_K can be arbitrarily chosen, it might be, in general, a function of q, p, and t. Then, we put

$$\epsilon^\alpha_K\equiv\epsilon^\beta(t)\rho^\alpha_\beta(q,p), \tag{3.4}$$

where $\epsilon^\beta(t)$ is an arbitrary function of t $(\beta=1\sim A)$. But G should also satisfy (2.9) by which the form of $\rho^\alpha_\beta(q,p)$ is restricted. The simplest form is $\rho^\alpha_\beta=\delta^\alpha_\beta$ and $\epsilon^\alpha_K=\epsilon^\alpha(t)$. This form is always allowed by adjusting a multicative function of ϕ^1_α.

Here, it should be noticed that even if we take in (2.16) as

$$\epsilon^\alpha_{(1)K}=\epsilon^\alpha_{(1)}(t),\quad\epsilon^\alpha_{(2)K}=\epsilon^\alpha_{(2)}(t), \tag{3.5}$$

$\epsilon^{\alpha}_{(3)K}$ turns to depend on q and p, if $C^{kl\gamma}_{\alpha\beta,m}$ and $C^{\beta}_{\alpha k}$ are dependent of q and p. Here, $G(\epsilon_{(3)})$ defined by (2.16) is guaranteed to satisfy (2.8) and (2.9), as already seen, owing to the Jacobi identity, even if $\epsilon^{\alpha}_{(3)K}$ is dependent of q and p.

Now let us derive explicit forms of ϵ^{α}_{k} $(k<K)$ using (3.2). By iteration, we successively find

$$\epsilon^{\alpha}_{K-1} = -\dot{\epsilon}^{\alpha} - C^{\alpha}_{\beta K}\epsilon^{\beta}, \quad \epsilon^{\alpha}_{K-2} = \ddot{\epsilon}^{\alpha} + C^{\alpha}_{\beta K}\dot{\epsilon}^{\beta} + (\dot{C}^{\alpha}_{\beta K} - C^{\alpha}_{\beta K-1})\epsilon^{\beta},$$

$$\vdots$$

$$\epsilon^{\alpha}_{K-l} = (-)^{l}\Big[\overset{(l)}{\epsilon}{}^{\alpha} + C^{\alpha}_{\beta K}\overset{(l-1)}{\epsilon}{}^{\beta} + \left\{\binom{l-1}{1}\dot{C}^{\alpha}_{\beta K} - C^{\alpha}_{\beta K-1}\right\}\overset{(l-2)}{\epsilon}{}^{\beta} + \left\{\binom{l-1}{2}\ddot{C}^{\alpha}_{\beta K} - \binom{l-2}{1}\dot{C}^{\alpha}_{\beta K-1} + C^{\alpha}_{\beta K-2}\right\}\overset{(l-3)}{\epsilon}{}^{\beta}$$
$$+ \left\{\binom{l-1}{3}\overset{(3)}{C}{}^{\alpha}_{\beta K} - \binom{l-2}{2}\ddot{C}^{\alpha}_{\beta K-1} + \binom{l-3}{1}\dot{C}^{\alpha}_{\beta K-2} - C^{\alpha}_{\beta K-3}\right\}\overset{(l-4)}{\epsilon}{}^{\beta} + \cdots + \Big\{\overset{(l-1)}{C}{}^{\alpha}_{\beta K} - \overset{(l-2)}{C}{}^{\alpha}_{\beta K-1}$$
$$+ \cdots + (-)^{l-2}\dot{C}^{\alpha}_{\beta K-l+2} + (-)^{l-1}C^{\alpha}_{\beta K-l+1}\Big\}\epsilon^{\beta}\Big], \tag{3.6}$$

where $\overset{(l)}{\epsilon}{}^{\alpha}_{k}$ and $\overset{(l)}{C}{}^{\alpha}_{\beta k}$ are defined by repeatedly applying (3.3) and

$$\dot{C}^{\alpha}_{\beta k} \equiv \frac{\partial C^{\alpha}_{\beta k}}{\partial t} + \{C^{\alpha}_{\beta k}, H\}. \tag{3.7}$$

From the Jacobi identity for ϕ^{k}_{α}, ϕ^{l}_{β}, and H, and using (2.4) and (2.5), it follows that

$$C^{kl\delta}_{\alpha\beta,m-1} + C^{kl\gamma}_{\alpha\beta,K}C^{\delta}_{\gamma m} - C^{k+1l\delta}_{\alpha\beta,m} + C^{l+1k\delta}_{\beta\alpha,m}$$
$$- \delta^{k}_{K}(C^{\gamma}_{\alpha n}C^{nl\delta}_{\gamma\beta,m} + \{C^{\delta}_{\alpha m}, \phi^{l}_{\beta}\}) + \delta^{l}_{K}(C^{\gamma}_{\beta n}C^{nk\delta}_{\gamma\alpha,m}$$
$$+ \{C^{\delta}_{\beta m}, \phi^{k}_{\alpha}\}) - \{H, C^{kl\delta}_{\alpha\beta,m}\} = D^{kl\delta\epsilon}_{\alpha\beta,mn}\phi^{n}_{\epsilon}, \tag{3.8}$$

with

$$D^{kl\delta\epsilon}_{\alpha\beta,mn} = -D^{kl\epsilon\delta}_{\alpha\beta,nm}, \tag{3.9}$$

which is an unknown function of q and p. The antisymmetry of D with respect to (δ,m) and (ϵ,n) is due to the even Grassmann parity of ϕ^{k}_{α}. For ϕ^{k}_{α} with the odd Grassmann parity, D is symmetry. The Jacobi identity among ϕ^{k}_{α}, ϕ^{l}_{β}, and ϕ^{m}_{γ} yields

$$C^{kl\delta}_{\alpha\beta,n}C^{nm\epsilon}_{\delta\gamma,s} + \{C^{kl\epsilon}_{\alpha\beta,s}, \phi^{m}_{\gamma}\} + (\text{cyclic sum on } {}^{klm}_{\alpha,\beta,\gamma})$$
$$= D^{klm\epsilon\delta}_{\alpha\beta\gamma,sn}\phi^{n}_{\delta}. \tag{3.10}$$

From (2.9), we obtain

$$\epsilon^{\beta}_{k}C^{1k\gamma}_{\alpha\beta,l} + \{\phi^{1}_{\alpha}, \epsilon^{\gamma}_{l}\} = E^{1\gamma\delta}_{\alpha,lm}\phi^{m}_{\delta} \quad (l\geqslant 2), \tag{3.11}$$

with

$$E^{1\gamma\delta}_{\alpha,lm} = -E^{1\delta\gamma}_{\alpha,ml}. \tag{3.12}$$

Equations (3.8), (3.10), and (3.11) are the conditions that should be satisfied by $C^{kl\gamma}_{\alpha\beta,m}$ and $C^{\beta}_{\alpha k}$.

Equations (3.8) and (3.11) play important roles. First, we determine $C^{1k\gamma}_{\alpha\beta,l}$ with the help of (3.11). Since ϵ^{α}_{K} is arbitrary, put

$$\epsilon^{\alpha}_{K} \equiv \epsilon^{\alpha}(t). \tag{3.13}$$

Then, (3.11) for $l=K$ gives

$$\epsilon^{\beta}_{k}C^{1k\gamma}_{\alpha\beta,K} \equiv E^{1\gamma\delta}_{\alpha,Km}\phi^{m}_{\delta} \quad (K\geqslant 2). \tag{3.14}$$

This relation is valid for $K\geqslant 2$, due to $l\geqslant 2$ in (3.11). Now, we assume ϵ^{α}_{k} to be independent of ϕ^{l}_{β} [note that ϵ^{α}_{k} may be dependent of q and p owing to (3.6), even $\epsilon^{\alpha}_{K} = \epsilon^{\alpha}(t)$]. Then, from (3.14), we are led to

$$C^{1k\gamma}_{\alpha\beta,K} = \overline{C}{}^{1k\gamma\delta}_{\alpha\beta,Km}\phi^{m}_{\delta}.$$

If $C^{kl\gamma}_{\alpha\beta,m}$ is linear homogeneous in ϕ^{k}_{α}, the right-hand side (rhs) of (2.6) takes the form $\overline{C}{}^{kl\gamma\delta}_{\alpha\beta,mn}\phi^{m}_{\gamma}\phi^{n}_{\delta}$ that is symmetric with respect to (γ,m) and (δ,n). Since the antisymmetric part of $\overline{C}{}^{kl\gamma\delta}_{\alpha\beta,mn}$ plays no role, it can be omitted. Thus we may put

$$E^{1\gamma\delta}_{\alpha,Km} = 0, \tag{3.15}$$

and

$$\epsilon^{\beta}_{k}C^{1k\gamma}_{\alpha\beta,K} = 0 \quad (K\geqslant 2). \tag{3.16}$$

The substitution of (3.6) into (3.16) leads to

$$\epsilon^{\beta}C^{1K\gamma}_{\alpha\beta,K} - (\dot{\epsilon}^{\beta} + C^{\beta}_{\delta K}\epsilon^{\delta})C^{1K-1\gamma}_{\alpha\beta,K}$$
$$+ (\ddot{\epsilon}^{\beta} + \dot{\epsilon}^{\delta}C^{\beta}_{\delta K} + \cdots)C^{1K-2\gamma}_{\alpha,\beta,K}\cdots$$
$$+ (-1)^{K-1}(\overset{(K-1)}{\epsilon}{}^{\beta} + \overset{(K-2)}{\epsilon}{}^{\delta}C^{\beta}_{\delta K} + \cdots)C^{11\gamma}_{\alpha\beta,K} = 0. \tag{3.17}$$

Since $\epsilon^{\alpha}(t)$ is arbitrary, all $\overset{(k)}{\epsilon}{}^{\alpha}(t)$ can be regarded as independent. In (3.17), $\overset{(K-1)}{\epsilon}{}^{\beta}$ appears only in the last term, hence,

$$C^{11\gamma}_{\alpha\beta,K} = 0.$$

In this way, we obtain, successively,

$$C^{1k\gamma}_{\alpha\beta,K} = 0 \quad (K\geqslant k\geqslant 1 \text{ and } K\geqslant 2). \tag{3.18}$$

Next, putting $l=K-1$ in (3.11) and using the first equation of (3.6), we find

$$\epsilon^{\beta}_{k}C^{1k\gamma}_{\alpha\beta,K-1} - \{\phi^{1}_{\alpha}, C^{\gamma}_{\beta K}\}\epsilon^{\beta} = E^{1\gamma\delta}_{\alpha,K-1m}\phi^{m}_{\delta} \quad (K\geqslant 3). \tag{3.19}$$

From the substitution of (3.6) into (3.19), it follows that, for $K\geqslant 3$,

$$C^{1k\gamma}_{\alpha\beta,K-1} = 0 \quad (k\leqslant K-1), \tag{3.20}$$

$$C^{1K\gamma}_{\alpha\beta,K-1} - \{\phi^{1}_{\alpha}, C^{\gamma}_{\beta K}\} \approx 0. \tag{3.21}$$

In (3.21), the weak equality $\approx$ indicates the contribution from the rhs of (3.19). The strong equality of (3.20) is due to the same reason as in (3.16). Similar relations are obtained by putting $l=K-2, K-3$ and so on. Summarizing them, we obtain

$$C^{1k\gamma}_{\alpha\beta,l} = 0 \quad (k \leqslant l, l \geqslant 2), \tag{3.22}$$

$$C^{1K-m+1\gamma}_{\alpha\beta,K-m} - \{\phi^1_\alpha, C^\gamma_{\beta K}\} \approx 0$$

$$(m = 1,2,\ldots,K-2; K \geqslant 3), \tag{3.23}$$

and

$$C^{1K-m+1\gamma}_{\alpha\beta,K-m-1} - C^\delta_{\beta K} C^{1K-m\gamma}_{\alpha\delta,K-m-1} + \{\phi^1_\alpha, m\dot{C}^\gamma_{\beta K} - C^\gamma_{\beta K-1}\} \approx 0,$$

$$(m = 1,2,\ldots,K-3; K \geqslant 4). \tag{3.24}$$

The relation (3.22) indicates that the stationarity conditions of ϕ^k_β using H_T of (2.3) yield no second class constraint, since the stationarity condition

$$\dot{\phi}^k_\beta = \phi^{k+1}_\beta - v^\alpha C^{1k\gamma}_{\alpha\beta,l}\phi^l_\gamma \approx 0$$

leads to $\phi^{k+1}_\beta \approx 0$ owing to (3.22). This result is consistent with the starting assumption that all constraints are first class. Based on these relations and (3.8), more general expressions of $C^{kl\gamma}_{\alpha\beta,m}$ are derived. A detail of the derivation is shown in the Appendix.

We have proved in the Appendix that

$$C^{kl\gamma}_{\alpha\beta,K} = 0 \quad (k \text{ or } l < K), \tag{3.25}$$

at least for $K \leqslant 4$, namely, only $C^{KK\gamma}_{\alpha\beta,K}$ is nonvanishing among $C^{kl\gamma}_{\alpha\beta,K}$. For $K > 5$, the proof is so complicated that we have not yet succeeded, although (3.25) seems, in general, to hold. We will then conjecture that (3.25) is true for all K. [For a practical use, (3.25) is sufficient with $K \leqslant 4$.]

The condition (3.25) leads us to the very important conclusion that the structure of the gauge group is almost determined only by $C^{KK\gamma}_{\alpha\beta,K}$.

IV. ALGEBRAIC STRUCTURES OF GAUGE GROUPS AND THEIR CLASSIFICATION

Since the generator $G(\epsilon_{(3)})$ defined by (2.16) satisfies (2.8) and (2.9), $\epsilon^\alpha_{(3)k}$ also satisfies (3.2). Hence, all $\epsilon^\alpha_{(3)k}$ are expressed in terms of $\epsilon^\alpha_{(3)K}$ and $G(\epsilon_{(3)})$ can be determined by $\epsilon^\alpha_{(3)K}$. From (2.16) and (2.17), it follows that

$$\begin{aligned}\epsilon^\alpha_{(3)k}\phi^k_\alpha &= \{\epsilon^\alpha_{(1)k}\phi^k_\alpha, \epsilon^\beta_{(2)l}\phi^l_\beta\} \\ &= \epsilon^\alpha_{(1)k}\epsilon^\beta_{(2)l}C^{kl\gamma}_{\alpha\beta,m}\phi^m_\gamma + \epsilon^\alpha_{(1)k}\{\phi^k_\alpha, \epsilon^\beta_{(2)l}\}\phi^l_\beta \\ &\quad + \epsilon^\beta_{(2)l}\{\epsilon^\alpha_{(1)k}, \phi^l_\beta\}\phi^k_\alpha + \{\epsilon^\alpha_{(1)k}, \epsilon^\beta_{(2)l}\}\phi^k_\alpha\phi^l_\beta.\end{aligned} \tag{4.1}$$

As all ϕ^k_α are independent, $\epsilon^\alpha_{(3)K}$ can be obtained by identifying the coefficients of ϕ^K_α in both sides of (4.1). Here, let $\epsilon^\alpha_{(1)K}$ and $\epsilon^\beta_{(2)K}$ be functions of t alone and assume $\{\epsilon^\alpha_k, \phi^l_\beta\}$ and $\{\epsilon^\alpha_{(1)k}, \epsilon^\beta_{(2)l}\}$ to contain no ϕ^K_γ. This assumption would be reasonable except for very special cases, as seen from the expressions (3.6) for ϵ^α_k. In the rhs of (4.1), ϕ^K_α remains only in the first term and we have

$$\epsilon^\gamma_{(3)K} = \epsilon^\alpha_{(1)k}\epsilon^\beta_{(2)l}C^{kl\gamma}_{\alpha\beta,K}. \tag{4.2}$$

In extracting (4.2) from (4.1), there may be an antisymmetric term similar to $D\dddot{\phi}$ in (3.8) or $E\dddot{\phi}$ in (3.11). Since such a term, however, disappears in constructing $G(\epsilon_{(3)}) = \epsilon^\gamma_{(3)k}\phi^k_\gamma$, we have omitted it.

Owing to (3.25), (4.2) reduces to

$$\epsilon^\gamma_{(3)K} = \epsilon^\alpha_{(1)}\epsilon^\beta_{(2)}C^{KK\gamma}_{\alpha\beta,K}, \tag{4.3}$$

with

$$\epsilon^\alpha_{(a)} \equiv \epsilon^\alpha_{(a)K}(t) \quad (a = 1,2).$$

Equation (4.3) is the very remarkable result to indicate that the structure of GT for parametrization ϵ^α can be specified only by $C^{KK\gamma}_{\alpha\beta,K}$. In other words, the algebraic structure of the gauge group is determined by the final step ϕ^K_α in the constraint series (2.4).

Further relations for $C^{kl\gamma}_{\alpha\beta,m}$ and $C^\beta_{\alpha k}$ can be derived from coefficients of ϕ^{K-1}_α, ϕ^{K-2}_α and so on in (4.1) (see the Appendix).

On the basis of the above observation, we can conclude that the types of the gauge groups can be classified in terms of (i) $C^{KK\gamma}_{\alpha\beta,K}$ and (ii) the number of the constraint step K.

In the first classification (i), we have three types.

(1) The case of $C^{KK\gamma}_{\alpha\beta,K} = 0$.

In this case, $\epsilon^\alpha_{(3)} = 0$, namely, $G(\epsilon_{(3)}) = 0$, so that the gauge group is Abelian. Hence, the gauge theory with a single gauge degree of freedom ($\alpha = \beta = 1$) is Abelian. The model in which all gauge degrees are completely isolated belongs to this type.

(2) The case of all $C^{KK\gamma}_{\alpha\beta,K} = \text{constant} \neq 0$.

Since $\epsilon^\alpha_{(3)}$ also is a function of t alone owing to (4.3), $G(\epsilon_{(3)})$ has the same form with $G(\epsilon_{(a)})$. Here $G(\epsilon)$'s close with respect to the Poisson bracket. The Yang–Mills theory[1] is of this type.

(3) The case of $C^{KK\gamma}_{\alpha\beta,K}$ being dependent of q and/or p.

Even $\epsilon^\alpha_{(a)}$ ($a = 1,2$) are functions of only t, $\epsilon^\alpha_{(3)}$ depends on q and/or p. Then $G(\epsilon)$ is not the generator of a Lie group (for t fixed).[8] $G(\epsilon)$'s do not close with respect to the Poisson brackets. By repeatation of the GT, new forms of δq^i appear successively, that is $G(\epsilon_{(3)})$ has a different form from the one of $G(\epsilon_{(a)})$. The generator X_E given by (2.25) is an example of this type. Though the calculation of the commutator of X_E is tedious, the Poisson bracket (2.16) for G is rather simple. Hence, we can regard G as a "generator" of the generator X_E.

For the case of $C^{KK\gamma}_{\alpha\beta,K}$ being dependent of q and/or p, a further classification would be needed, basing on a detailed observation. For instance, there would be an essential difference according to whether $C^{KK\gamma}_{\alpha\beta,K}$ contains p or not.

A typical example of the case (3) is the relativistic membrane with $n(\geqslant 2)$ spatial dimensions.[9]

In the classification (ii) in terms of K, the number of the constraint steps, we can derive more precise conclusion with the help of informations concerning $C^\beta_{\alpha k}$ (the structure functions of $\{\phi^K_\alpha, H\}$).

(1) The case of $K = 1$.

No specific consequence is derived in the case where only the primary constraints appear, since the relations obtained in Sec. III and the Appendix are available for the case of $K \geqslant 2$.

(2) The case of $K = 2$.

Most of gauge field theories (e.g., electromagnetic, Yang–Mills, and gravitational fields, etc.) belong to the type. As shown in (A40), we have

$$C^{11\gamma}_{\alpha\beta,1} = C^{1k\gamma}_{\alpha\beta,2} = 0 \quad (k = 1,2), \tag{4.4}$$

$$2C^{12\gamma}_{\alpha\beta,1} = 2C^{12\gamma}_{\beta\alpha,1} = \{\phi^1_\alpha, C^\gamma_{\beta 2}\} + \{\phi^1_\beta, C^\gamma_{\alpha 2}\}, \tag{4.5}$$

$$2C^{22\gamma}_{\alpha\beta,1} \approx C^\delta_{\alpha 2} C^{12\gamma}_{\beta\delta,1} - C^\delta_{\beta 2} C^{12\gamma}_{\alpha\delta,1} - \{\phi^1_\alpha, C^\gamma_{\beta 1}\} + \{\phi^1_\beta, C^\gamma_{\alpha 1}\}, \tag{4.6}$$

and

$$2C^{22\gamma}_{\alpha\beta,2} = -\{\phi^1_\alpha, C^\gamma_{\beta 2}\} + \{\phi^1_\beta, C^\gamma_{\alpha 2}\} = 2C^{12\gamma}_{\alpha\beta,1} - 2\{\phi^1_\alpha, C^\gamma_{\beta 2}\}. \tag{4.7}$$

From (4.7), we obtain

$$C^{22\gamma}_{\alpha\beta,2} = 0, \tag{4.8}$$

if

$$\{\phi^1_\alpha, C^\gamma_{\beta 2}\} - \{\phi^1_\beta, C^\gamma_{\alpha 2}\} = 0. \tag{4.9}$$

Then, the gauge group is Abelian. Further, if

$$C^\beta_{\alpha 1} = C^\beta_{\alpha 2} = \text{constant}, \tag{4.10}$$

all

$$C^{kl\gamma}_{\alpha\beta,m} = 0. \tag{4.11}$$

These are remarkable results.

In the Yang–Mills theory where (4.9) is not satisfied and $C^\beta_{\alpha 2} = f^\beta_{\alpha\gamma} A^\gamma_0(x)$, we have [except for the factor $\delta(\mathbf{x}-\mathbf{y})$]

$$C^{22\gamma}_{\alpha\beta,2} = f_{\alpha\beta}{}^\gamma \text{ (the structure constant of the group)} \tag{4.12}$$

and all other $C^{kl\gamma}_{\alpha\beta,m} = 0$. Equations (4.4)–(4.7) suggest the possibility of

$$C^{12\gamma}_{\alpha\beta,1} \neq 0 \text{ or } C^{22\gamma}_{\alpha\beta,1} \neq 0, \tag{4.13}$$

which is a type different from the Yang–Mills theory. Furthermore, even for the Abelian case $C^{22\gamma}_{\alpha\beta,2} = 0$, we cannot exclude the case of (4.13); i.e.,

$$C^{12\gamma}_{\alpha\beta,1} \neq 0 \text{ or } C^{22\gamma}_{\alpha\beta,1} \neq 0.$$

(3) The case of $K = 3$.

Omitting the derivation, we present only useful relations;

$$C^{12\gamma}_{\alpha\beta,k} = C^{12\gamma}_{\beta\alpha,k} \quad (k = 1,2), \tag{4.14}$$

$$C^{12\gamma}_{\alpha\beta,1} = -C^{31\gamma}_{\alpha\beta,2}, \tag{4.15}$$

and

$$C^{33\gamma}_{\alpha\beta,3} = C^{23\gamma}_{\alpha\beta,2} - \{\phi^2_\alpha, C^\gamma_{\beta 3}\} = -\frac{1}{2} C^{22\gamma}_{\alpha\beta,1} - \frac{1}{2}\{\phi^2_\alpha, C^\gamma_{\beta 3}\} + \frac{1}{2}\{\phi^2_\beta, C^\gamma_{\alpha 3}\}. \tag{4.16}$$

It is observed in (4.16) that $C^{33\gamma}_{\alpha\beta,3} \neq 0$, that is, non-Abelian even if $C^\beta_{\alpha 3} = \text{constant}$. This is contrast to the case of $K = 2$.

V. DISCUSSION

In this paper, we have shown that the algebraic structure and the property of the gauge group is essentially determined by FCCs of the final step of constraint series appearing in their stationarity conditions. The classification of the gauge groups can be made in terms of the property of $C^{KK\gamma}_{\alpha\beta,K}$ and the number of the constraint steps K, as shown in Sec. IV. Here, we emphasize that our definition (2.4) and (2.5) of the constraint series are crucial in order to obtain such a simple conclusion. The consequences obtained will be useful for analysis of the properties of gauge groups.

Remained problems are as follows: (i) to prove (3.25) for $K \geqslant 5$, (ii) to apply our formulation to physically interesting models, (iii) to find new types of gauge theories, and (iv) to remove the assumption for $\{\epsilon^\alpha_k, \phi^l_\beta\}$ and $\{\epsilon^\alpha_{(1)k}, \epsilon^\beta_{(2)l}\}$ to contain no ϕ^k_γ.

APPENDIX: RELATIONS HOLDING AMONG $C^{kl\gamma}_{\alpha\beta,m}$'S AND $C^\beta_{\alpha k}$'S.

First of all, we will derive (3.25). From (3.8) for $m = K$, $k = 1$ and (3.18), it follows that

$$C^{1l\delta}_{\alpha\beta,K-1} - C^{2l\delta}_{\alpha\beta,K} = D^{1l\delta\epsilon}_{\alpha\beta,Km}\phi^m_\epsilon \approx 0. \tag{A1}$$

Owing to (3.20), (A1) reduces to

$$C^{1l\gamma}_{\alpha\beta,K-1} = C^{2l\gamma}_{\alpha\beta,K} = 0 \quad (l < K), \tag{A2}$$

where the exact equality is due to the reason same with those for (3.15) and (3.16). By putting $m = l = K$ and $k = 1$ in (3.8), we have

$$C^{1K\gamma}_{\alpha\beta,K-1} - C^{2K\gamma}_{\alpha\beta,K} + \{C^\gamma_{\beta K}, \phi^1_\alpha\} \approx 0, \tag{A3}$$

which yields, with the help of (3.21),

$$C^{2K\gamma}_{\alpha\beta,K} = 0 \quad (K \geqslant 3). \tag{A4}$$

Combining (3.18), (A2) and (A4), we obtain

$$C^{1k\gamma}_{\alpha\beta,K} = C^{2k\gamma}_{\alpha\beta,K} = 0 \quad (k = 1 \sim K, K \geqslant 3). \tag{A5}$$

Thus only $C^{3k\gamma}_{\alpha\beta,K}$ can be nonzero for $K \geqslant 3$.

Next, let us prove for $K \geqslant 4$

$$C^{3K\gamma}_{\alpha\beta,K} = 0. \tag{A6}$$

Equation (3.8) reduces to, for $m = K-1$, $k = 2$, and $l < K$,

$$C^{2l\gamma}_{\alpha\beta,K-1} \approx C^{3l\gamma}_{\alpha\beta,K} \quad (l < K), \tag{A7}$$

owing to (A5) and $C^{kl\gamma}_{\alpha\beta,m} = -C^{lk\gamma}_{\beta\alpha,m}$. From (3.8), for $m = K-1$, $k = 1$, $l < K$, and (3.18), we find

$$C^{1l\gamma}_{\alpha\beta,K-2} - C^{2l\gamma}_{\alpha\beta,K-1} - C^{1l+1\gamma}_{\alpha\beta,K-1} \approx 0 \tag{A8}$$

in which for $l \leqslant K-2$, the first and the third terms vanish due to (3.18). Further, for $l = K-1$, the first and third terms in (A8) cancel each other, owing to the relation

$$C^{1K-1\gamma}_{\alpha\beta,K-2} - C^{1K\gamma}_{\alpha\beta,K-1} \approx 0 \quad (K \geqslant 4), \tag{A9}$$

which is obtained from (3.23). Consequently, we get

$$C^{2l\gamma}_{\alpha\beta,K-1} = 0 \quad (l < K, K \geqslant 4). \tag{A10}$$

Equations (A7) and (A10) give

$$C^{3l\gamma}_{\alpha\beta,K} = 0 \quad (l < K, K \geqslant 4). \tag{A11}$$

In order to obtain (A11) for $l = K$, we put $m = K-1$, $k = 1$, and $l = K$ in (3.8) to get

$$C^{1K\delta}_{\alpha\beta,K-2} - C^{2K\delta}_{\alpha\beta,K-1} + C^\gamma_{\beta K} C^{K1\delta}_{\gamma\alpha,K-1} + \{C^\delta_{\beta K-1}, \phi^1_\alpha\} - \{H, C^{1K\delta}_{\alpha\beta,K-1}\} \approx 0. \tag{A12}$$

The last term of (A12) turns out to be $-\{H, [\phi^1_\alpha, C^\delta_{\beta K}]\}$ by using (3.23). On the other hand, with the help of (3.23), (3.24) for $m = 1$ becomes

$$C^{1K\delta}_{\alpha\beta,K-2} - C^\gamma_{\beta K} C^{1K\delta}_{\alpha\gamma,K-1} + \{C^\delta_{\beta K-1}, \phi^1_\alpha\} + \{\phi^1_\alpha, [C^\delta_{\beta K}, H]\} \approx 0. \tag{A13}$$

Hence, (A12) and (A13) yield

$$C^{2K\gamma}_{\alpha\beta,K-1} \approx -\{C^{\gamma}_{\beta K},[\phi^1_\alpha H]\} = -\{C^{\gamma}_{\beta K},\phi^2_\alpha\} \quad (K\geqslant 4). \tag{A14}$$

In the above derivation, the Jacobi identity and (2.4) have been used. Again, putting $m = l = K$ and $k = 2$ in (3.8), we obtain

$$C^{2K\gamma}_{\alpha\beta,K-1} - C^{3K\gamma}_{\alpha\beta,K} + \{C^{\gamma}_{\beta K},\phi^2_K\} \approx 0. \tag{A15}$$

From (A14) and (A15), (A6) follows. Thus (A6) and (A11) are combined to give

$$C^{3k\gamma}_{\alpha\beta,K} = 0 \quad (k = 1\sim K, K\geqslant 4). \tag{A16}$$

Consequently, only $C^{KK\gamma}_{\alpha\beta,K}$ can be nonvanishing among $C^{kl\gamma}_{\alpha\beta,K}$ for $K\leqslant 4$.

For $K\geqslant 5$, the proof is so complicated that we have not succeeded in it. But we conjecture, for any K

$$C^{kl\gamma}_{\alpha\beta,K} = 0 \quad (k \text{ or } l < K). \tag{A17}$$

By the way, the substitution of (A17) into (3.10) with $s = K$ gives

$$\begin{aligned} &\{C^{KK\gamma}_{\alpha\beta,K},\phi^l_\gamma\} \approx 0 \quad (l < K), \\ &\{C^{KK\delta}_{\alpha\beta,K},C^{KK\epsilon}_{\delta\gamma,K}\} + \{C^{KK\epsilon}_{\alpha\beta,K},\phi^K_\gamma\} \approx 0. \end{aligned} \tag{A18}$$

From (4.1), other expressions of $C^{kl\gamma}_{\alpha\beta,m}$ for $m \neq K$ can be derived. From the coefficient of ϕ^{K-1}_α in (4.1), the following relation is derived:

$$\begin{aligned} \epsilon^{\gamma}_{(3)K-1} = {} & \epsilon^{\alpha}_{(1)k}\epsilon^{\beta}_{(2)l}C^{kl\gamma}_{\alpha\beta,K-1} + \epsilon^{\alpha}_{(1)k}\{\phi^k_\alpha,\epsilon^{\gamma}_{(2)K-1}\} \\ & + \epsilon^{\beta}_{(2)k}\{\epsilon^{\gamma}_{(1)K-1},\phi^k_\beta\} + \{\epsilon^{\gamma}_{(1)K-1},\epsilon^{\beta}_{(2)l}\}\phi^l_\beta \\ & + \{\epsilon^{\alpha}_{(1)k},\epsilon^{\gamma}_{(2)K-1}\}\phi^k_\alpha. \end{aligned} \tag{A19}$$

Due to the first equation of (3.6), (A19) reduces to

$$\begin{aligned} -\dot\epsilon^{\gamma}_{(3)} - C^{\gamma}_{\beta K}\epsilon^{\beta}_{(3)} = {} & \epsilon^{\alpha}_{(1)k}\epsilon^{\beta}_{(2)l}C^{kl\gamma}_{\alpha\beta,K-1} \\ & - \{\epsilon^{\alpha}_{(1)k}\phi^k_\alpha,C^{\gamma}_{\beta K}\}\epsilon^{\beta}_{(2)} \\ & + \{\epsilon^{\alpha}_{(2)k},\phi^k_\alpha,C^{\gamma}_{\beta K}\}\epsilon^{\beta}_{(1)}, \end{aligned} \tag{A20}$$

where $\epsilon^{\alpha}_{(a)} \equiv \epsilon^{\alpha}_{(a)K}$ $(a = 1,2)$ are put to be independent of q and p. By substituting the expressions of (3.6) into ϵ^{α}_k in (A.20), there appear $\overset{(K-k)}{\epsilon}{}^{\alpha}_{(1)}$, $\overset{(K-k-1)}{\epsilon}{}^{\alpha}_{(1)}$,..., while in the left-hand side (lhs) only the first-order time derivative of $\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)}$ exist, owing to (4.3). In the rhs of (A20), the coefficients of $\overset{(r)}{\epsilon}{}^{\alpha}_{(1)}\overset{(s)}{\epsilon}{}^{\beta}_{(2)}$ $(r,s\geqslant 1)$ should then vanish;

$$C^{kl\gamma}_{\alpha\beta,K-1} = 0 \text{ (both } k \text{ and } l\leqslant K-1; K\geqslant 2). \tag{A21}$$

Hence, only $C^{kK\gamma}_{\alpha\beta,K-1}$ can survive.

Since the highest derivative $\overset{(K-1)_\alpha}{\epsilon}{}_{(1)}$ comes out from $\epsilon^{\alpha}_{(1)1}$, we have for the coefficient of $\epsilon^{\beta}_{(2)}$ in (A20)

$$C^{1K\gamma}_{\alpha\beta,K-1} - \{\phi^1_\alpha,C^{\gamma}_{\beta k}\} = 0 \quad (K\geqslant 3). \tag{A22}$$

Since the term $\overset{(K-2)_\alpha}{\epsilon}{}_{(1)}$ appears from $\epsilon^{\alpha}_{(1)1}$ and $\epsilon^{\alpha}_{(1)2}$, the following relation holds:

$$\begin{aligned} & C^{\delta}_{\alpha K}C^{1K\gamma}_{\delta\beta,K-1} - C^{2K\gamma}_{\alpha\beta,K-1} - \{C^{\delta}_{\alpha K}\phi^1_\delta,C^{\gamma}_{\beta K}\} \\ & \quad + \{\phi^2_\alpha,C^{\gamma}_{\beta K}\} = 0 \quad (K\geqslant 4). \end{aligned} \tag{A23}$$

With the help of (A22), (A23) reduces to

$$C^{2K\gamma}_{\alpha\beta,K-1} + \{C^{\delta}_{\alpha K},C^{\gamma}_{\beta K}\}\phi^1_\delta - \{\phi^2_\alpha,C^{\gamma}_{\beta K}\} = 0. \tag{A24}$$

Also, from (A15) and (A24), it follows that

$$\{C^{\delta}_{\alpha K},C^{\gamma}_{\beta K}\}\phi^1_\delta = D^{2K\gamma\delta}_{\alpha\beta,Km}\phi^m_\delta \quad (K\geqslant 4), \tag{A25}$$

hence,

$$\begin{aligned} & \{C^{\delta}_{\alpha K},C^{\gamma}_{\beta K}\} = D^{2K\gamma\delta}_{\alpha\beta,K1} \quad (K\geqslant 4), \\ & C^{2K\gamma}_{\alpha\beta,K-1} - \{\phi^2_\alpha,C^{\gamma}_{\beta K}\} = -D^{2K\gamma\delta}_{\alpha\beta,K1}\phi^1_\delta. \end{aligned} \tag{A26}$$

From the coefficient of ϕ^{K-2}_α in (4.1), we find

$$C^{kl\gamma}_{\alpha\beta,K-2} = 0 \begin{pmatrix} k\leqslant K-1, & l\leqslant K-2 \\ \text{or } k\leqslant K-2, & l\leqslant K-1 \end{pmatrix}. \tag{A27}$$

Since it is so tedious to obtain further relations for arbitrary K, we will apply the above method to the case of $K = 2$ and find useful relations. Now, we have

$$\epsilon^{\gamma}_{(3)} = C^{22\gamma}_{\alpha\beta,2}\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)}. \tag{A28}$$

The substitution of

$$\epsilon^{\alpha}_{(.)1} = -\dot\epsilon^{\alpha}_{(.)} - C^{\alpha}_{\beta 2}\epsilon^{\beta}_{(.)}$$

into (A19) for $K = 2$ yields

$$\begin{aligned} & -\dot C^{22\gamma}_{\alpha\beta,2}\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)} - C^{22\gamma}_{\alpha\beta,2}(\dot\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(1)} + \epsilon^{\alpha}_{(1)}\dot\epsilon^{\beta}_{(2)}) - C^{\gamma}_{\delta 2}C^{22\delta}_{\alpha\beta,2}\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)} \\ & = [C^{22\gamma}_{\alpha\beta,1} - \{\phi^2_\alpha,C^{\gamma}_{\beta 2}\} + \{\phi^2_\beta,C^{\gamma}_{\alpha 2}\} + \{C^{\gamma}_{\alpha 2},C^{\delta}_{\beta 2}\phi^1_\delta\} - \{C^{\gamma}_{\beta 2},C^{\delta}_{\alpha 2}\phi^1_\delta\} - C^{\delta}_{\alpha 2}C^{12\gamma}_{\delta\beta,1} + C^{\delta}_{\beta 2}C^{12\gamma}_{\delta\alpha,1}] \\ & \quad \times\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)} + [-C^{12\gamma}_{\alpha\beta,1} + \{\phi^1_\alpha,C^{\gamma}_{\beta 2}\}]\dot\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{2} + [C^{12\gamma}_{\alpha\beta,1} - \{\phi^1_\alpha,C^{\gamma}_{\beta 2}\}]\epsilon^{\beta}_{(1)}\dot\epsilon^{\alpha}_{(2)}. \end{aligned} \tag{A29}$$

The coefficient of $\dot\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)}$ in (A29) yields

$$C^{22\gamma}_{\alpha\beta,2} = C^{12\gamma}_{\alpha\beta,1} - \{\phi^1_\alpha,C^{\gamma}_{\beta 2}\}, \tag{A30}$$

and from the antisymmetric part of $\epsilon^{\alpha}_{(1)}\epsilon^{\beta}_{(2)}$ with respect to α and β, it follows that

$$\begin{aligned} \dot C^{22\gamma}_{\alpha\beta,2} + C^{\gamma}_{\delta 2}C^{22\delta}_{\alpha\beta,2} = {} & -C^{22\gamma}_{\alpha\beta,1} + C^{\delta}_{\alpha 2}C^{12\gamma}_{\delta\beta,1} - C^{\delta}_{\beta 2}C^{12\gamma}_{\delta\alpha,1} \\ & + \{\phi^2_\alpha,C^{\gamma}_{\beta 2}\} - \{\phi^2_\beta,C^{\gamma}_{\alpha 2}\} \\ & + \{C^{\gamma}_{\alpha 2},C^{\delta}_{\beta 2}\phi^1_\delta\} - \{C^{\gamma}_{\beta 2},C^{\delta}_{\alpha 2}\phi^1_\delta\}. \end{aligned} \tag{A31}$$

With the use of (A30), (A31) turns out to be

$$\begin{aligned} & \dot C^{22\gamma}_{\alpha\beta,2} + C^{\gamma}_{\delta 2}C^{22\delta}_{\alpha\beta,2} + C^{22\gamma}_{\alpha\beta,1} - C^{\delta}_{\alpha 2}C^{22\gamma}_{\delta\beta,2} + C^{\delta}_{\beta 2}C^{22\gamma}_{\delta\alpha,2} \\ & \quad - \{\phi^2_\alpha,C^{\gamma}_{\beta 2}\} + \{\phi^2_\beta,C^{\gamma}_{\alpha 2}\} + (\{C^{\gamma}_{\alpha 2},C^{\delta}_{\beta 2}\} \\ & \quad - \{C^{\gamma}_{\beta 2},C^{\delta}_{\alpha 2}\})\phi^1_\delta = 0. \end{aligned} \tag{A32}$$

On the other hand, (3.8) with $k = l = m = 2$ becomes

$$\begin{aligned} & C^{22\gamma}_{\alpha\beta,1} + C^{22\delta}_{\alpha\beta,2}C^{\gamma}_{\delta 2} - C^{\delta}_{\alpha 2}C^{22\gamma}_{\delta\beta,2} + C^{\delta}_{\beta 2}C^{22\gamma}_{\delta\alpha,2} \\ & \quad - \{C^{\gamma}_{\alpha 2},\phi^2_\beta\} + \{C^{\gamma}_{\beta 2},\phi^2_\alpha\} + \dot C^{22\gamma}_{\alpha\beta,2} \approx 0. \end{aligned} \tag{A33}$$

Then from (A32) and (A33), it follows that

$$\{C^{\gamma}_{\alpha 2},C^{\delta}_{\beta 2}\} \approx \{C^{\gamma}_{\beta 2},C^{\delta}_{\alpha 2}\}. \tag{A34}$$

Again putting $k=l=m=1$ in (3.8) and using (3.22), we obtain

$$C^{21\delta}_{\alpha\beta,1} = C^{21\delta}_{\beta\alpha,1}. \tag{A35}$$

The α,β antisymmetric part of (A30) reduces to

$$2C^{22\delta}_{\alpha\beta,2} = -\{\phi^1_\alpha, C^\delta_{\beta 2}\} + \{\phi^1_\beta, C^\delta_{\alpha 2}\} \tag{A36}$$

with the help of (A35), and the α,β symmetric part to

$$2C^{12\gamma}_{\alpha\beta,1} = \{\phi^1_\alpha, C^\gamma_{\beta 2}\} + \{\phi^1_\beta, C^\gamma_{\alpha 2}\}. \tag{A37}$$

Equation (3.8) with $k=m=1$ and $l=2$, turns out to be

$$-C^{22\delta}_{\alpha\beta,1} + C^\gamma_{\beta 2} C^{21\delta}_{\gamma\alpha,1} + \{C^\delta_{\beta 1}, \phi^1_\alpha\} + \dot{C}^{21\delta}_{\alpha\beta,1} \approx 0. \tag{A38}$$

The α,β antisymmetric part of (A38) gives

$$2C^{22\delta}_{\alpha\beta,1} \approx -C^\gamma_{\beta 2} C^{12\delta}_{\alpha\gamma,1} + C^\gamma_{\alpha 2} C^{12\delta}_{\beta\gamma,1} - \{\phi^1_\alpha, C^\delta_{\beta 1}\} + \{\phi^1_\beta, C^\delta_{\alpha 1}\}. \tag{A39}$$

Summarizing all results obtained for $K=2$, we have

$$C^{11\gamma}_{\alpha\beta,1} = C^{1k\gamma}_{\alpha\beta,2} = 0,$$

$$2C^{12\gamma}_{\alpha\beta,1} = 2C^{12\gamma}_{\beta\alpha,1} = \{\phi^1_\alpha, C^\gamma_{\beta 2}\} + \{\phi^1_\beta, C^\gamma_{\alpha 2}\},$$

$$2C^{22\gamma}_{\alpha\beta,1} \approx C^\delta_{\alpha 2} C^{12\gamma}_{\beta\delta,1} - C^\delta_{\beta 2} C^{12\gamma}_{\alpha\delta,1} - \{\phi^1_\alpha, C^\gamma_{\beta 1}\} + \{\phi^1_\beta, C^\gamma_{\alpha 1}\},$$

$$2C^{22\gamma}_{\alpha\beta,2} = -\{\phi^1_\alpha, C^\gamma_{\beta 2}\} + \{\phi^1_\beta, C^\gamma_{\alpha 2}\} = 2C^{12\gamma}_{\alpha\beta,1} - 2\{\phi^1_\alpha, C^\gamma_{\beta 2}\}, \tag{A40}$$

$$\{C^\gamma_{\alpha 2}, C^\delta_{\beta 2}\} \approx \{C^\gamma_{\beta 2}, C^\delta_{\alpha 2}\},$$

and

$$\epsilon^\gamma_{(3)} = C^{22\gamma}_{\alpha\beta,2} \epsilon^\alpha_{(1)} \epsilon^\beta_{(2)}.$$

The weak equality $\approx$ means the existence of a contribution from the $D\phi$ or $E\phi$ term as in (3.8) or (3.12).

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Symmetrized powers of the fundamental irrep of E_6

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The resolution of all possible antisymmetrically symmetrized powers of the fundamental irrep (**27**) is given. This reduces the problem of plethysms of the fundamental irrep to the evaluation of ordinary Kronecker products of E_6 irreps.

I. INTRODUCTION

The group E_6 has been of considerable interest to particle model builders[1] and more recently we[2] have found it relevant to interacting boson models (IBM) involving s, d, g, i bosons. In each case, the 27-dimensional fundamental irrep of E_6 plays a key role. In the case of the IBM, the resolution of symmetrized powers of the fundamental irrep is required. This problem is equivalent to the evaluation of the branching rules for $SU_{27} \rightarrow E_6$ where the vector irrep $\{\mathbf{1}\}$ reduces as $\{\mathbf{1}\} \rightarrow (\mathbf{27})$.

II. THEORY

The irreps of E_6 may be variously labeled. In much of the physics literature, the irreps have been simply labeled by quoting their dimensions and using primes (') to distinguish distinct irreps of the same dimension and underlines and overbars to distinguish an irrep and its conjugate,[1] e.g., ($\underline{\mathbf{27}}$) and ($\overline{\mathbf{27}}$). More precise labeling comes from the use of the corresponding labels based ony the maximal $SU_2 \times SU_6$ subgroup of E_6, the so-called *natural labeling*.[3–5] In that scheme the irreps of E_6 are labeled as $(s{:}\lambda)$ where s is an integer label for SU_2 and λ is a constrained partition such that

$$s \geqslant \lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 - \lambda_5$$

and the weight of λ is *even*. The labels $(s{:}\lambda)$ are related to the corresponding Dynkin labels $(a_1 a_2 a_3 a_4 a_5 a_6)$ by[4]

$$\begin{aligned}
s &= a_1 + 2a_2 + 3a_3 + 2a_4 + a_5 + 2a_6,\\
\lambda_1 &= a_1 + a_2 + a_3 + a_4 + a_5,\\
\lambda_2 &= a_2 + a_3 + a_4 + a_5,\\
\lambda_3 &= a_3 + a_4 + a_5,\\
\lambda_4 &= a_4 + a_5,\\
\lambda_5 &= a_5.
\end{aligned}$$

In terms of the natural labeling the fundamental irrep of E_6 is designated as (1:1) and its conjugate irrep as (1:11111).

Using the earlier results of Wybourne and Bowick[3] together with King's method[6] for evaluating E_6 Kronecker products it was possible to adapt the program SCHUR to compute and verify $SU_{27} \rightarrow E_6$ branching rules given in Table I.

The characters of SU_{27} can be represented in terms of Schur functions in the roots of the defining group elements and hence there is a one-to-one correspondence between the partitions that label an SU_{27} irrep and those labeling the appropriate Schur function. Furthermore, any Schur function $\{\lambda\}$ can be expanded as a sum of products of Schur functions $\{1^x\}$ and hence Table I permits every plethysm of the fundamental irrep of E_6 to be reduced to the evaluation of Kronecker products of the E_6 irreps that occur in Table I. These can be readily evaluated using King's algorithm[6] and the $E_6 \rightarrow SU_2 \times SU_6$ branchings that are all known. Thus we have a complete and systematic procedure for constructing arbitrary plethysms of the fundamental irrep of E_6.

TABLE I. Antisymmetric powers of the fundametal irrep (1:1) of E_6.

Dimension	$SU_{27} \rightarrow E_6$	
1	$\{0\}$	(0:0)
27	$\{1\}$	(1:1)
351	$\{1^2\}$	(2:11)
2925	$\{1^3\}$	(3:111)
17550	$\{1^4\}$	(4:1111)
80730	$\{1^5\}$	(5:11111) + (4:2222)
296010	$\{1^6\}$	(6:0) + (5:22221)
888030	$\{1^7\}$	(6:1111) + (5:33322)
2220075	$\{1^8\}$	(6:22211) + (5:44333)
4686825	$\{1^9\}$	(6:33222) + (6:222) + (5:54444)
8436285	$\{1^{10}\}$	(6:43333) + (6:33211) + (5:55555)
13037895	$\{1^{11}\}$	(6:44444) + (6:43322) + (6:3311)
17383860	$\{1^{12}\}$	(6:44433) + (6:43221) + (6:33)
20058300	$\{1^{13}\}$	(6:44332) + (6:43111) + (6:4222)

Given that[7] $(A \otimes B) \otimes C = A \otimes (B \otimes C)$ it follows that any irrep of E_6 that can be expressed as a sum of products of plethysms of the fundamental irrep can be readily evaluated. For example, since $(1{:}1) \otimes \{1^2\} = (2{:}11)$ it follows that

$$\begin{aligned}
(2{:}11) \otimes \{\lambda\} &= ((1{:}1) \otimes \{1^2\}) \otimes \{\lambda\}\\
&= (1{:}1) \otimes (\{1^2\} \otimes \{\lambda\}).
\end{aligned}$$

Thus we conclude that a complete and systematic method is available for determining arbitrary plethysms of the fundamental irrep of E_6 and furthermore can simplify other E_6 plethysms. We have used the above results to readily evaluate the plethysms of the fundamental irrep of E_6 for all partitions of weight $\leqslant 8$.

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Algebras for the two-sphere and the three-sphere groups of compact simple Lie groups

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The infinite-dimensional Lie algebras corresponding to the Lie groups of smooth maps from two and three spheres to compact simple Lie groups are studied. The problem of their central extension is solved. The problem of the existence of semidirect sum algebras containing these and the algebras of the groups of diffeomorphisms on the two and three spheres is treated.

I. INTRODUCTION

Some time ago, Bars[1] studied the structure of the two-sphere algebra associated with a Lie group. Homotopically trivial smooth maps from a two-sphere S^2 to a Lie group G form a certain infinite parameter group under point-wise multiplication. The corresponding infinite-dimensional Lie algebra is the two-sphere algebra associated with G. The concept of the two-sphere algebra is an extension of the idea of the loop algebra—the algebra of the group of homotopically trivial smooth maps from a circle to a Lie group. The central extension of the loop algebra is the Kac–Moody algebra.[2,3] The latter has found wide applications in physics.[4] Groups of maps from d-spheres S^d to compact Lie groups and their associated algebras are expected to find useful physical applications. For one thing, these structures appear naturally in the study of current algebras. Indeed, it is motivated by considerations of current algebras that Mickelsson and Rajeev[5] were led to the problem of constructing highest weight representations of d-sphere groups. Moreover, sphere groups and algebras are expected to prove useful in the description of spatially extended objects with extension in more than one spatial dimension (membrane theories). This is in analogy with the role of the Kac–Moody algebras in string theories. For all these reasons, as also for the sake of its intrinsic merit, it appears worthwhile to pursue the study of these structures as a purely mathematical enterprise.

This paper is addressed to several features of sphere algebras. First, we shall write down the commutation relations of the three-sphere algebra—the Lie algebra of maps: $S^3 \to G$, S^3 a three-sphere, G a Lie group. This task, of course, is absolutely straightforward. Secondly, and this is the main result of this paper, we shall carry out the central extension of the two-sphere and three-sphere algebras of a compact, simple Lie group G. Finally, we shall make some comments on the structure of these algebras.

As far as the two-sphere algebra is concerned, Bars[1] has already considered the problem of its central extension. But his treatment is incomplete. He wrote down a two-term central extension, whereas it will be shown in the sequel that the algebra has an infinite number of central extensions. This, indeed, must be the case according to a general theorem proved by Feigin.[6] Let us recall the Feigin result. Let M be a manifold and G a compact Lie group with g the corresponding Lie algebra. Let g^M denote the Lie algebra of the group of maps: $M \to G$. By a standard procedure[7] one constructs an algebraic complex associated with g^M, which is contained in the de Rham complex of the corresponding group. Let $H^2(g^M)$ denote the second cohomology group of g^M. Then the Feigin result states that $H^2(g^M)$ is infinite dimensional whenever the manifold M has a dimension greater than 1. Since the space $H^2(g^M)$ has the interpretation as a set of classes of one-dimensional central extensions of g^M, the implication is that the algebra g^M possesses an infinite number of independent central extensions whenever the dimension of the manifold M is greater than 1. The set of solutions for the central extensions that we obtain is found to contain one of the two terms written down by Bars.[1] The other term, upon closer scrutiny, will be found to be unacceptable.

This paper is organized as follows. In Sec. II we write the basic commutation relations of the three-sphere algebra. In Sec. III, the problem of central extensions of the two and three-sphere algebras is solved. The significance of the results obtained is next analyzed in terms of the anomalies in the current algebra in Sec. IV. The final Sec. V contains discussions and comments.

II. ALGEBRAS

Let G be a Lie group, g the Lie algebras of G, T^a the elements of a basis for g, and f^{abc} the corresponding structure constants [a, b, c run from 1 to dim (g)]. We denote by g^M the Lie algebra of the group of (homotopically trivial, smooth) maps: $M \to G$. Here, our interest is confined to the two cases $M = S^2$ and $M = S^3$. A basis for g^M is provided by operators of the form $T_L{}^a$. When $M = S^2$, L stands for the ordered pair (l,m), l is a non-negative integer and allowed values of m range from $-l$ to $+l$, changing in steps of one. For the case $M = S^3$, L stands for the ordered triple (l,m,m'), and here both m and m' separately have the same spectrum as in the previous case but l is now a non-negative integer or half-integer. We shall also be making use of the subscript notation; thus $T_{L_1}{}^a$ would stand for $T^a{}_{l_1 m_1}$ or $T^a{}_{l_1 m_1 m'_1}$ depending on the context.

For the two-sphere algebra the basic commutation relations is[1]

$$[T^a{}_{L_1}, T^b{}_{L_2}] = f^{abc} C(L_1, L_2; L) T^c{}_L, \tag{1}$$

where

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$$C(L_1,L_2;L) = \langle l_1 m_1, l_2 m_2 | lm \rangle \langle l_1 0, l_2 0 | l 0 \rangle \times [(2l_1+1)(2l_2+1)/4\pi(2l+1)]^{1/2} \quad (2)$$

and terms in brackets that appear above are the standard Clebsch–Gordan coefficients. Equation (2) is derivable from the "defining representation" $T^a_L \equiv T^a Y_{lm}$, where $Y_{lm}(\theta,\phi)$ are the spherical harmonics that provide a complete set of basis functions for any L^2 integrable function on the two-sphere. Furthermore,

$$Y_{l_1 m_1}(\theta,\phi) Y_{l_2 m_2}(\theta,\phi) = C(L_1,L_2;L) Y_{lm}(\theta,\phi) \quad (3)$$

is the expansion of a product into a sum. It should be noted that there is a summation over the dummy index L, that is, over l and m in Eq. (1), with the range of summation being restricted by the non-vanishing properties of the coefficient function given by Eq. (2). Actually, a repeated index will always imply an appropriate summation.

The analog of Eq. (1) for the three-sphere algebra may now be obtained. The manifold S^3 is parametrized by the Euler angles α, β, γ, the rotation matrices $D^l_{mm'}(\alpha,\beta,\gamma)$ provide a complete basis for functions on S^3 (from the Peter–Weyl theorem) and the analog of Eq. (3) for the product of the two rotation matrices is given by the celebrated Clebsch–Gordan expansion for the group SU(2). Thus we find that in the present instance the basic commutation relation can still be written formally, exactly as Eq. (1); only this time the coefficient function is different and is given by

$$C(L_1,L_2;L) = \langle l_1 m_1, l_2 m_2 | lm \rangle \langle l_1 m_1', l_2 m_2' | lm' \rangle, \quad (4)$$

where the brackets, once again, are Clebsch–Gordan coefficients.

III. CENTRAL EXTENSIONS

We shall now treat the problem of central extension of the two algebras that we have considered in the preceding section. Let us write the basic commutation relations for the centrally extended algebra in the form

$$[T^a_{L_1}, T^b_{L_2}] = f^{abc} C(L_1,L_2;L) T^c_L + d^{ab}_{L_1,L_2(A)} K^A \quad (5)$$

where K^A are the central generators that commute with each other and with all the T^a_L generators:

$$[K^A, K^B] = 0, \quad [K^A, T^a_L] = 0. \quad (6)$$

In the above, A is an index that labels the independent central elements; the precise nature of this index will be made clear in the sequel. We shall often suppress this index on the term $d^{ab}_{L_1,L_2}$ for the sake of notational convenience. The Jacobi identity as applied to the commutator Eq. (5) leads to

$$f^{abd} C(L_1,L_2;L) d^{dc}_{L,L_3} + f^{bcd} C(L_2,L_3;L) d^{da}_{L,L_1} + f^{cad} C(L_3,L_1;L) d^{db}_{L,L_2} = 0, \quad (7)$$

where a summation over the dummy indices d and L is understood. Notice that the range of L summation is different for each of the three terms in Eq. (7), and is controlled by the nonvanishing properties of the coefficient functions. Equation (7) is the cocycle condition, its solutions will yield the desired central extensions. However, some of these are trivial in the sense of being coboundaries. These can be eliminated by a suitable change of basis. We seek nontrivial solutions of Eq. (7). It is clear that such solutions form a vector space. This is the second cohomology vector space of the sphere algebra.

At this stage, we restrict our Lie group G to be compact and simple. We can now choose the basis for g in which the structure constants are completely antisymmetric and obey

$$f^{abc} f^{abd} = \delta^{cd}. \quad (8)$$

Combining Eqs. (7) and (8), we have

$$C(L_1,L_2;L) d^{ab}_{L,L_3} + f^{cda} f^{dbe} C(L_2,L_3;L) d^{ec}_{L,L_1} + f^{dca} f^{bde} C(L_3,L_1;L) d^{ec}_{L,L_2} = 0. \quad (9)$$

Taking now, $L_2 = 0$, $L_3 = 0$ in Eq. (9) and utilizing the Jacobi relations for the structure constants f^{abc} of g and the antisymmetry property $d^{ab}_{L_1,L_2} = -d^{ba}_{L_2,L_1}$, we derive

$$d^{ab}_{L_1,0} = f^{abd} f^{ced} d^{ce}_{L_1,0}. \quad (10)$$

On the other hand, Eq. (7) is unchanged under the transformation

$$T^a_L \to T^a_L + \xi^a_{L,A} K^A, \quad (11)$$

under which the central terms behave as

$$d^{ab}_{L_1,L_2(A)} \to d^{ab}_{L_1,L_2(A)} - f^{abc} C(L_1,L_2;L) \xi^c_{L,A}, \quad (12)$$

where $\xi^a_{L,A}$ are certain functions. Using Eq. (12) we can set $d^{ab}_{L_1,0}$ to zero, for such a and b for which f^{abc} does not vanish identically. In the event f^{abc} does vanish, Eq. (10) says that $d^{ab}_{L_1,0}$ vanish also. Thus, quite generally, we can set

$$d^{ab}_{L,0} = 0. \quad (13)$$

Thus T^a_0 generate a subalgebra isomorphic with the original Lie algebra g and the T^a_L transform as the adjoint representation of g, for each L. This conclusion follows from Eq. (5). Taking now $L_2 = 0$ in Eq. (7) and using Eq. (13) and the fact $C(0,L_1;L) = C(L_1,0;L) \sim \delta_{L_1,L}$ we get:

$$f^{bad} d^{dc}_{L_1,L_3} + f^{bcd} d^{ad}_{L_1,L_3} = 0, \quad (14)$$

which is recognized to be the condition that $d^{ab}_{L_1,L_3}$ is an isotropic tensor under the action of g. From this, it follows that the dependence on the indices a and b must be of the form δ^{ab}. This is exactly as it happens[4] with the loop algebra. Thus we set

$$d^{ab}_{L_1,L_2} = \delta^{ab} d_{L_1,L_2} \quad (15)$$

and Eq. (7) reduces to

$$C(L_1,L_2;L) d_{L,L_3} + C(L_2,L_3;L) d_{L,L_1} + C(L_3,L_1;L) d_{L,L_2} = 0. \quad (16)$$

The above equation plus antisymmetry $d_{L_1,L_2} = -d_{L_2,L_1}$ determine the central extension terms. We proceed to construct solutions to Eq. (16).

Let us first treat the case of the two-sphere algebra. The coefficient function $C(L_1,L_2;L)$ is here given by Eq. (2). Consider the derivative of the product of three spherical harmonics:

$$\partial_i \{Y_{L_1}(\theta,\phi) Y_{L_2}(\theta,\phi) Y_{L_3}(\theta,\phi)\} = C(L_1,L_2;L) Y_L(\theta,\phi) \partial_i Y_{L_3}(\theta,\phi)$$

$$+ C(L_2,L_3;L)\,Y_L(\theta,\phi)\partial_i Y_{L_1}(\theta,\phi)$$
$$+ C(L_3,L_1;L)\,Y_L(\theta,\phi)\partial_i Y_{L_2}(\theta,\phi), \qquad (17)$$

where $i = 1,2; \partial_1 \equiv \partial/\partial\phi$ and $\partial_2 \equiv \partial/\partial z$ and $z = \cos\theta$. In deriving the above result, Eq. (3) has been used. From Eq. (17) we obtain

$$(\partial_2 Y_{L'})\partial_1(Y_{L_1}Y_{L_2}Y_{L_3}) - (\partial_1 Y_{L'})\partial_2(Y_{L_1}Y_{L_2}Y_{L_3}) = C(L_1,L_2;L)\,Y_L\left[(\partial_2 Y_{L'})(\partial_1 Y_{L_3}) - (\partial_1 Y_{L'})(\partial_2 Y_{L_3})\right]$$
$$+ C(L_2,L_3;L)\,Y_L\left[(\partial_2 Y_{L'})(\partial_1 Y_{L_1}) - (\partial_1 Y_{L'})(\partial_2 Y_{L_1})\right]$$
$$+ C(L_3,L_1;L)\,Y_L\left[(\partial_2 Y_{L'})(\partial_1 Y_{L_2}) - (\partial_1 Y_{L'})(\partial_2 Y_{L_2})\right]. \qquad (18)$$

Now for any pair (L', L) it is true, as is easily verified, that

$$\int \left[(\partial_2 Y_{L'})(\partial_1 Y_L) - (\partial_1 Y_{L'})(\partial_2 Y_L)\right] d\Omega = 0, \qquad (19)$$

where $d\Omega = dz\,d\phi/4\pi$. Since we can express the product of three Y's as a linear combination of Y's, it now follows that if we integrate both sides of (18) over the two-sphere then the left-hand side must vanish. The resulting equation is then compared with Eq. (16) to obtain the desired central elements. We thus arrive at

$$d_{L_1,L_2(L)} \equiv d_{L_1,L_2} = \int Y_{l_1 m_1} D_L Y_{l_2 m_2} d\Omega, \qquad (20)$$

where

$$D_L \equiv D_{lm} = \left(\frac{\partial Y_{lm}}{\partial z}\right)\frac{\partial}{\partial\phi} - \left(\frac{\partial Y_{lm}}{\partial\phi}\right)\frac{\partial}{\partial z}. \qquad (21)$$

The independent central extensions are labeled by L and as before $z = \cos\theta$. In writing the above equations, we reverted back to a more conventional notation. It is instructive to note the central terms for $l = 1$; these are

$$d_{L_1,L_2(10)} = (-1)^{m_1} m_1 \delta_{m_1+m_2,0}\delta_{l_1,l_2}, \qquad (22)$$

$$d_{L_1,L_2(1,\pm 1)} = (-1)^{m_1}\sqrt{l_1(l_1+1) - m_1(m_1 \pm 1)} \times \delta_{m_1+m_2\pm 1,0}\delta_{l_1,l_2} \qquad (23)$$

Let us now solve Eq. (16) for the case of the three-sphere algebra, i.e., when the coefficient function $C(L_1,L_2;L)$ is given by Eq. (4). The derivation of the central terms proceeds much the same way as in the previous case and it, therefore, seems quite pointless to keep on writing the messy algebraic expressions that arise in this exercise. The essential point is this. There are now three variables α, β, and γ in contrast to two of the earlier case. Correspondingly, we can write three distinct relations analogous to Eq. (18), by taking the pairings (α, z), (z, γ), and (γ, α); here $z = \cos\beta$. Consequently, we shall obtain a triply infinite set of solutions to Eq. (16). These are found to be

$$d^i_{L_1,L_2(L)} = \int D^{l_1}_{m_1 m_1'}(\alpha,\beta,\gamma) D^i_L D^{l_2}_{m_2 m_2'}(\alpha,\beta,\gamma) d\Omega, \qquad (24)$$

where $d\Omega$ is the Haar measure on S^3 and

$$D^1_L \equiv D^1_{lmm'} = \left(\frac{\partial D^l_{mm'}}{\partial\gamma}\right)\frac{\partial}{\partial z} - \left(\frac{\partial D^l_{mm'}}{\partial z}\right)\frac{\partial}{\partial\gamma},$$

$$D^2_L \equiv D^2_{lmm'} = \left(\frac{\partial D^l_{mm'}}{\partial\alpha}\right)\frac{\partial}{\partial\gamma} - \left(\frac{\partial D^l_{mm'}}{\partial\gamma}\right)\frac{\partial}{\partial\alpha},$$

$$D^3_L \equiv D^3_{lmm'} = \left(\frac{\partial D^l_{mm'}}{\partial z}\right)\frac{\partial}{\partial\alpha} - \left(\frac{\partial D^l_{mm'}}{\partial\alpha}\right)\frac{\partial}{\partial z}. \qquad (25)$$

Here $z = \cos\beta$ and independent central terms are labeled by $i(= 1,2,3)$ and $L = (l,m,m')$. We should note that the central elements given by Eqs. (20) and (24) satisfy Eq. (13), which is necessary for consistency.

IV. CURRENT ALGEBRAS

Let us construct "currents" via

$$T^a(\theta,\phi) = \sum_L T^a_L Y_L(\theta,\phi). \qquad (26)$$

The above is for the two-sphere; for the three-sphere replace the spherical harmonics by the rotation matrix element $D^l_{mm'}(\alpha,\beta,\gamma)$. The commutation relation Eq. (1) gets converted into the current algebra commutation relations for the currents $T^a(\theta,\phi)$ or $T^a(\alpha,\beta,\gamma)$, whereas the central extension terms [Eq. (5)] become anomalies. Thus the basic commutator relations have the structure

$$[T^a(x), T^b(x')] = f^{abc}\delta(x-x')T^c(x') + \text{anomaly}. \qquad (27)$$

What is the anomaly corresponding to the central terms that we found in the preceeding section? Let us investigate this question for the two cases separately; first, for the two-sphere. For this case let us write the anomaly in Eq. (27) in the following form:

$$\delta^{ab}\left[f_1(\theta,\phi)\delta(z-z')\delta'(\phi-\phi') + f_2(\theta,\phi)\delta'(z-z')\delta(\phi-\phi')\right], \qquad (28)$$

where, f_1 and f_2 are two functions on $S^2, z = \cos\theta$ and the delta prime δ' is the derivative of the Dirac delta function δ. Indeed, the Jacobi identity, as applied to Eqs. (27) and (28), is easily shown to lead to the condition

$$\frac{\partial f_1}{\partial\phi} + \frac{\partial f_2}{\partial z} = 0. \qquad (29)$$

The solution of the above, on S^2, is

$$f_1(\theta,\phi) = \frac{\partial}{\partial z}h(\theta,\phi), \quad f_2(\theta,\phi) = -\frac{\partial}{\partial\phi}h(\theta,\phi), \qquad (30)$$

where $h(\theta,\phi)$ is an arbitrary function on S^2. Using Eqs. (26) and (27) if we now compute the central term d_{L_1,L_2} arising out of the expressions in Eq. (30), by expanding $h(\theta,\phi)$ into spherical harmonics we then find for d_{L_1,L_2} exactly the expression in Eqs. (20) and (21). The infinite number of central elements thus correspond to the infinite number of

components of the function $h(\theta,\phi)$ on the $Y_{lm}(\theta,\phi)$ basis.

The foregoing discussion is extended to the three-sphere algebra as follows. The anomaly term in this case is written in the following form:

$$\delta^{ab}[f_1\delta(z-z')\delta(\gamma-\gamma')\delta'(\alpha-\alpha')+f_2\delta'(z-z')\times\delta(\gamma-\gamma')\delta(\alpha-\alpha')+f_3\delta(z-z')\times\delta'(\gamma-\gamma')\delta(\alpha-\alpha')], \tag{31}$$

where f_1, f_2, and f_3 are certain functions on S^3. The Jacobi relation now leads to the condition

$$\frac{\partial}{\partial\alpha}f_1+\frac{\partial}{\partial z}f_2+\frac{\partial}{\partial\gamma}f_3=0. \tag{32}$$

The solution of Eq. (32), on S^3, is given by a set of three functions h_1, h_2, and h_3, as follows

$$\begin{aligned} f_1&=\frac{\partial}{\partial z}h_3-\frac{\partial}{\partial\gamma}h_2,\\ f_2&=\frac{\partial}{\partial\gamma}h_1-\frac{\partial}{\partial\alpha}h_3,\\ f_3&=\frac{\partial}{\partial\alpha}h_2-\frac{\partial}{\partial z}h_1. \end{aligned} \tag{33}$$

In the above, $z=\cos\beta$ and α,β,γ are the Euler angles. If we now, using the above, construct the central terms, we find precisely the expression given in Eqs. (24) and (25).

At this stage we should compare our results with that of Bars.[1] He wrote down an expression for the anomaly that corresponds to the choice $f_1(\theta,\phi)=a$ and $f_2(\theta,\phi)=b$ in expression (28); here a and b are two constants. The term $f_1(\theta,\phi)=a$ corresponds to our Eq. (22) and to this extent our results agree. However, the other term $f_2(\theta,\phi)=b$ should not be there, since this term, despite its appearance to the contrary, is not properly antisymmetric and b must be set equal to zero. To see this, let us calculate the central element corresponding to the term $f_2(\theta,\phi)=b$. We obtain

$$d_{L_1,L_2}=\frac{b}{2}\left[\frac{(l_1-m_1)!(l_2-m_2)!}{(l_1+m_1)!(l_2+m_2)!}\right]^{1/2}\times[(2l_1+1)(2l_2+1)]^{1/2}\delta_{m_1+m_2,0}\times\int_{-1}^{1}dz\,P_{l_2}^{m_2}(z)\frac{d}{dz}P_{l_1}^{m_1}(z) \tag{34}$$

where P_l^m is the associated Legendre polynomial. Consider now the special case $m_1=0$ and the integral in Eq. (34) is not necessarily antisymmetric with respect to the exchange $l_1\leftrightarrow l_2$, since

$$\int_{-1}^{1}dz\,P_{l_2}(z)\frac{d}{dz}P_{l_1(z)}+\int_{-1}^{1}dz\,P_{l_1}(z)\frac{d}{dz}P_{l_2}(z)=1-(-1)^{l_1+l_2} \tag{35}$$

and antisymmetry fails to be true if $l_1+l_2=$ odd. The point is this: The delta prime (generalized) function is really the derivative operator. The *representation* of this operator fails to be properly antisymmetric since it acts on functions P_l that do not necessarily enjoy the property $P_l(+1)=P_l(-1)$.

V. REMARKS

Consider the question of inclusions; if the three-sphere algebra, Eqs. (1) and (4), contains the two-sphere algebra, Eqs. (1) and (2), and if the latter contains the loop algebra (the Kac–Moody algebra modulo its center)? From inspection of Eqs. (2) and (4), it is immediate that the answer to the first question is in the affirmative. Indeed, generators T_L^a with L of the form $L=(l,m,0)$ and $L=(l,0,m')$ separately span two isomorphic copies of the two-sphere algebra. As regards the second question, we note that operators T_L^a with $L=(l,l)$ lead to the commutation relation

$$\begin{aligned} &[T_{l_1}^a,T_{l_2}^b]=f^{abc}T_{l_1+l_2}^c,\\ &T_l^a=[4\pi/(2l+1)!]^{1/2}l!T_{ll}^a, \end{aligned} \tag{36}$$

as is easy to verify from Eqs. (1) and (2). The above is only one-half the loop algebra, since l here is restricted to a non-negative spectrum, $l\geqslant 0$. Note also, that T_L^a with $L=(l,-l)$ generate an isomorphic copy of Eq. (36) but these two isomorphic subalgebras do not commute with each other.

Do the foregoing conclusions continue to be true for the corresponding centrally extended algebras? The answer to this question turns out to be in the negative. The central elements in the commutators for the set T_L^a, with $L=(l,m,o)$, of operators, computed from Eq. (25), is found not to coincide with the desired central elements [Eq. (20)] for the extended two-sphere algebra. To settle the remaining issue, we compute using Eqs. (20) and (21), the central elements $d_{l_1,L_2(L)}$ with $L_1=(l_1,l_1)$, $L_2=(l_2,l_2)$ and find that these vanish for each L. Thus the commutator of operators $T_L^a\equiv T_{ll}^a$ continues to be given by Eq. (36).

Another question that should be entertained concerns the existence of grading operators. While these for the indices m and m' in T_{lm}^a and $T_{lmm'}^a$ can obviously be constructed, none exists for the index l. It is essentially for this reason that it is not possible to give a description of these algebras in terms of a *finite-dimensional* root vector space. This is a point of significant distinction between these algebras and the Kac–Moody algebra.

The final point of enquiry is based on an analogy. In the case of mapping of a circle, one has two structures: the Kac–Moody and the Virasoro algebra. It is further known that these two can be combined into a larger Lie algebra with the structure of a semidirect sum in which the Kac–Moody algebra appears as an ideal. Is a similar construction possible in the present instance? Now, for the spheres S^2 and S^3, the analog of the Virasoro algebra are,[8-10] respectively, diff(S^2) and diff(S^3)—the algebras of the group of diffeomorphisms of S^2 and S^3. Let us consider the case S^2 in some detail. The algebra diff(S^2) is generated by

$$L_L\equiv L_{lm}=\left(\frac{\partial Y_{lm}}{\partial z}\right)\frac{\partial}{\partial\phi}-\left(\frac{\partial Y_{lm}}{\partial\phi}\right)\frac{\partial}{\partial z}, \tag{37}$$

that satisfy

$$[L_{L_1},L_{L_2}]=f_{L_1,L_2}^{L}L_L. \tag{38}$$

In the above, $z=\cos\theta$ and expressions for the structure constants f_{L_1,L_2}^{L} have been given by Hoppe.[11] For our purpose it is useful to take note of the relation

$$\{Y_{L_1}, Y_{L_2}\} = f^L_{L_1,L_2} Y_L, \tag{39}$$

where the left-hand side of the above denotes a Poisson bracket (with respect to z and ϕ). Using Eqs. (37) and (39) and the "defining representation" $T^a_L \equiv T^a Y_L \equiv T^a Y_{lm}$, we obtain the commutator

$$[L_{L_1}, T^a_{L_2}] = f^L_{L_1,L_2} T^a_L, \tag{40}$$

which clearly shows the semidirect sum structure. The only question that now remains is the one of consistency, i.e., if all the relevant Jacobi identities are satisfied. It is obvious from Eqs. (38) and (40) that the Jacobi relation for the triple $(L_{L_1}, T^a_{L_2}, L_{L_3})$ is indeed fulfilled. What about the triple $(L_{L_1}, T^a_{L_2}, T^b_{L_3})$? Using Eqs. (5) and (40), plus the condition

$$[K^A, L_L] = 0, \tag{41}$$

we compute

$$\begin{aligned}[[L_{L_1}, T^a_{L_2}], T^b_{L_3}] + [[T^a_{L_2}, T^b_{L_3}], L_{L_1}] \\ + [[T^b_{L_3}, L_{L_1}], T^a_{L_2}] \\ = f^{abc} X(L_1 L_2 L_3 L') T^c_{L'} \\ + \delta^{ab} Y(L_1 L_2 L_3 L') K^{L'},\end{aligned} \tag{42}$$

where

$$\begin{aligned}X(L_1 L_2 L_3 L') = f^L_{L_1,L_2} C(L, L_3; L') - f^{L'}_{L_1,L} C(L_2, L_3; L) \\ + f^L_{L_1,L_3} C(L_2, L; L')\end{aligned} \tag{43}$$

and

$$Y(L_1 L_2 L_3 L') = f^L_{L_1,L_2} d_{L,L_3(L')} + f^L_{L_3,L_1} d_{L,L_2(L')}. \tag{44}$$

Applying the operator L_{L_1} to the product $Y_{L_2} Y_{L_3}$ and using Eq. (3), it is easily shown that

$$X(L_1 L_2 L_3 L') = 0. \tag{45}$$

On the other hand, $Y(L_1 L_2 L_3 L)$ is, in general, nonvanishing. We can easily convince ourselves of this by computing one particular case; say $L_1 = (1,1)$. $L_{1,1}$ is[12] (up to an inessential constant) the conventional angular momentum raising operator L_+ and the expression for the structure constant in Eq. (40) is now very simple. We can now immediately see that the corresponding Y is nonzero. Thus the conclusion is that there does not exist a larger algebra containing diff(S^2) and the *centrally extended* two-sphere algebra. However, such a structure does exist for diff(S^2) and the noncentrally extended two-sphere algebra. This conclusion can be extended to the case where the three-sphere algebra (or its central extension) is combined with the algebra diff(S^3) whose structure has been elucidated in Ref. 10. The proof runs parallel to that of the foregoing example and will, therefore, be omitted. Our last conclusion, it should be noted, is stable with respect to any possible central extension of diff(S^3) [diff(S^2) is known not to admit any central extension[13]]. Because of the semidirect sum structure, Eq. (40), any possible central element in the commutator of two L operators never enters the Jacobi identity.

It has been brought to our attention by the Referee that a general result concerning the classification of central extensions of the algebra g^M of the group of maps has been given by Pressley and Segal.[14] Let M be a compact manifold with dim$(M) > 1$, let G be a compact, simple Lie group and g^M the Lie algebra of the group of smooth maps: $M \to G$. The result of Pressley and Segal is this: central extensions correspond to the elements of the space $\Omega^1/d\Omega^0$ of one-forms on M modulo exact one-forms. To understand how our results relate to this general theorem, we proceed as follows. First, we note that a general one-form on M can be, by the Hodge decomposition theorem, written uniquely as a sum of an exact, a coexact, and a harmonic one-form. There are no harmonic one-forms on a sphere S^n $(n > 1)$, and thus for these cases the decomposition reduces to a sum of an exact and a coexact piece. It follows that each equivalence class of one-forms modulo exact one-forms contains a unique coexact representative. Thus the result of Pressley and Segal may be paraphrased to read that *central extensions are labeled by coexact one-forms on M in the case where M is a sphere.* The connection of this result with our work is most transparent if we look at the expressions for the anomaly in our current algebra. The functions f_i that appear in Eqs. (28) and (31) can be identified with the components, in a local system of coordinates, of a one-form f. Equations (30) and (33) correspond to the statement that f is coexact. For instance, Eq. (30) may be written as $f = \delta\beta$ where $f = f_1(1-z^2)d\phi + f_2(1-z^2)^{-1} dz$ and $\beta = h\, d\phi \wedge dz$. Note also that Eqs. (29) and (32) mean that f is coclosed, $\delta f = 0$, which is true. Thus our result is in complete agreement with that stated by Pressley and Segal. We may develop this theme further in order to gain additional insight. Thus our anomaly is the Lie derivative of the delta function with respect to the vector field

$$X = \sum_i f_i \frac{\partial}{\partial x^i},$$

here x^i are local coordinates such as ϕ and z on S^2 or α, z and γ on S^3. The corresponding expression for the Kac–Moody current algebra is d/dt, where t denotes the coordinate on a circle. The vector field X can always be interpreted as the pushforward of d/dt by a certain smooth map $\Phi: S^1 \to M$ given by $t \to x^i$, with $dx^i/dt = f_i$.

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Rough surfaces and the renormalization group

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Perturbative techniques are used to derive a renormalization group equation for a free scalar field in a domain with rough boundaries and mixed boundary conditions. It is found that to second order in the surface height the boundary conditions scale not only as the perturbed area, but also with a nonlinear term that arises from matching orders of surface height in the perturbation series for the field amplitude.

I. INTRODUCTION

Of late, many papers have been published on the subject of fractal-like surfaces. Experimental evidence for fractal-like surfaces such as sandstone, other geological and biological objects has been observed by use of absorption,[1] x-ray,[2] and NMR[3] techniques. But the more general question of how the introduction of a rough (fractal-like) surface affects a scalar field, has not been fully addressed.

Our approach is to solve Laplace's and Helmholtz's equation in the presence of a rough surface. The scalar field is assumed to obey mixed boundary conditions

$$[\hat{\mathbf{n}}\cdot\nabla\psi + f_0(S)\psi]_S = \left[\frac{\partial\psi}{\partial n} + f_0\psi\right]_S = g_0(S). \quad (1.1)$$

The cases $g_0(S) = 0$ and $f_0(S) = f_0$, independent of S is used for the bulk of this work. The process can be thought of as absorption, reflection, or any process described sufficiently by a scalar field. In this case, S will be the real physical surface and will be modeled in Sec. II as a "cutoff fractal." But it is also assumed that in the vicinity of S, there exists another surface S_0 such that $S_0 \in C^\infty$ and as $S \to S_0$ the problem is completely solvable.

We start here at S_0, the unperturbed boundary and by the methods outlined in Secs. II and III, we let $S_0 \to S$. A redefinition of f_0 is obtained, i.e., $f_0 \to f(S)$, where $f(S)$ is some undetermined surface parameter. An average over all possible samples gives a new boundary condition of the ensemble averaged field so that

$$\left[\frac{\partial\langle\psi\rangle}{\partial n_0} + f\langle\psi\rangle\right]_{S_0} = 0. \quad (1.2a)$$

In essence, we solve the boundary value problem at S_0 with the constraint

$$\left[\frac{\partial\psi}{\partial n_0} + f_0\psi\right]_S = 0. \quad (1.2b)$$

A differential equation for the transformation $f_0 \to f$ is found. This renormalization group equation (RGE) and its solution in terms of averaged surface parameters is the focus of this and subsequent papers.

A priori one expects three scenarios, as the surface changes from a smooth (C^∞) surface to a fractal (C^0) one.

Scenario 1: $f \to 0$. The boundary conditions become von Neumann at S_0 and the average behavior of the field can be solved as such.

Scenario 2: $f \to \infty$. In this case the averaged fields obey Dirichlet conditions.

Scenario 3: The renormalization proceeds to some value of f_0, possibly indeterminate, and the boundary conditions remain mixed if a fixed point is found. In the case of an indeterminate value for f, the problem under consideration may, in fact, be ill-posed. This very point will be the topic of future papers and is probably the most interesting possibility, for this would imply that no solution could be found for a true fractal boundary value problem as the cut-off is removed.

In Sec. II we introduce the concept of a cutoff fractal, the average or covariance and how they relate to the Hausdorf dimension. Section III describes in detail the perturbation techniques used to find the RGE. Sections IV and V are calculations of the solutions to second order in ϵ in both semiinfinite and the closed systems. These calculations provide some evidence that the basic form of the RGE may, in fact, be universal. Section VI provides a rough guess of the scale of the renormalization for the case of hydrodynamic diffusion in sandstone, along with discussion of future goals.

II. SURFACES AND STATISTICS

In many physical problems one encounters the concept of boundary conditions. In general, the actual shape of the boundary is idealized to be some regular geometrical object, usually taken to be a plane, cylinder, sphere, or some combination of the three. The operative word here is, "idealized," since in most physical applications real surfaces are rough. Our aim is to determine the behavior of systems when the boundary shape is not idealic.

Suppose the surfaces S, $S_0 \subset X^N$ (X^N some embedding space) are defined as follows [$\mathbf{x}_\parallel \equiv (x_1, x_2, \ldots, x_{N-1})$].

Definition 1—Boundaries S_0 and S:

$$S_0 = \{x \in X^N | x = (x_1, x_2, \ldots, x_{N-1}, h(x_1, x_2, \ldots, x_{N-1}))$$
such that $\epsilon h(\mathbf{x}_\parallel) = \text{const}\},$

$$S = \{x \in X^N | x = (x_1, x_2, \ldots, x_{N-1}, h(x_1, x_2, \ldots, x_{N-1}))\}.$$

For concreteness, the definitions of self-similar scale transformation (SSST) and scale-invariant surface (SIS) are the

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following definitions.[4]

Definition 2—Self-similar scale transformation (SSST): An SSST is a mapping of $r:S\to rS$, such that if $\mathbf{x}\in S$, then

$$r:\mathbf{x}\to r\mathbf{x}, \quad r\in\mathbf{R}, \text{ by the rule } r\mathbf{x}=(rx_1,\ldots,rx_N).$$

Definition 3—Scale-invariance: A surface is SIS if $\forall$ continuous $A\subset S\ \exists r\in\mathbf{R}$ such that $rA\cong S$.

Intuitively, Definition 3 states that one cannot distinguish between being on A or S, because with finite resolution both A and S exhibit the same characteristics. And by the same token this is what makes the surface non-Riemannian, because given any point $\mathbf{x}\in S$ there will be some scale, possibly infinite, at which the tangent space at $\mathbf{x}(TS_{\mathbf{x}})$ is not uniquely defined. Stated more simply, it would be impossible to smooth out all wiggles, bumps, overhangs, and depressions. In this sense a true fractal is infinitely rough. The simple act of limiting the scales of invariance will allow us to limit these points to a set of measure zero, i.e., given $\mathbf{x}\in B\subset S/\exists TS_{\mathbf{x}}$, then $\mu(B)=0$. Thus $h(\mathbf{x}_\parallel)$ is C^1 for $\mathbf{x}\in S/B$ one can define the tangent plane to S at point $(x_1,\ldots,x_{N-1},h(x_1,\ldots,x_{N-1}))$ in a natural way, as just the projection map φ:

$$\varphi:S\to TS_{\mathbf{x}}\cong\mathbf{R}^{N-1}, \quad \varphi(\mathbf{x})=x_\parallel.$$

Obviously this would be absurd to have a scale-invariant surface as a boundary, since one does not observe this sort of behavior at scales smaller than say a few Å, nor larger than the system under consideration. It is then reasonable to consider the system "cutoff" from these scales, and coin the term cutoff-fractal to describe this sort of surface.

Considering only those functions $h(\mathbf{x}_\parallel)$ in Definition 1, such that, $h(\mathbf{x}_\parallel)\in\mathscr{L}^2$ we proceed by defining the Fourier transform of $h(\mathbf{x}_\parallel)$:

$$h(\mathbf{x}_\parallel)=\int d^{N-1}\mathbf{q}_\parallel e^{-i\mathbf{q}_\parallel\cdot\mathbf{x}_\parallel}\tilde{h}(\mathbf{q}_\parallel),$$

$$\tilde{h}(\mathbf{q}_\parallel)=\frac{1}{(2\pi)^{N-1}}\int d^{N-1}\mathbf{x}_\parallel e^{i\mathbf{q}_\parallel\cdot\mathbf{x}_\parallel}h(\mathbf{x}_\parallel). \tag{2.1}$$

Easily stated, we expect that $h(\mathbf{x}_\parallel)$, and hence S can be adequately described by a two-point correlation function, or the covariance. The h's are assumed to be governed by Gaussian statistics, with zero mean height. Lastly, demanding translational invariance requires the covariance to be only a function of distance and not direction, while at the same time, maintaining the constant volume. These restrictions require

$$\langle h(\mathbf{x}_\parallel)\rangle=0 \text{ and } \langle h(\mathbf{x}_\parallel)h(\mathbf{y}_\parallel)\rangle=\xi(|\mathbf{x}_\parallel-\mathbf{y}_\parallel|), \tag{2.2}$$

where ξ, the "correlation function," is some function of the absolute value of the difference of position vectors $\mathbf{x}_\parallel$ and $\mathbf{y}_\parallel$. This has an important effect on the type of systems we may consider by requiring $\mathscr{G}$, the corresponding Fourier transformed averages, the power spectrum, to be an even function in $\mathbf{q}$ space. The transformed averages are then given by

$$\langle\tilde{h}(\mathbf{q}_\parallel)\rangle=0, \text{ and } \langle\tilde{h}(\mathbf{q}_\parallel)\tilde{h}(\mathbf{q}'_\parallel)\rangle=\delta(\mathbf{q}_\parallel+\mathbf{q}'_\parallel)\mathscr{G}(\mathbf{q}_\parallel), \tag{2.3}$$

where to cut off the scales of the surface $\mathscr{G}$ is assumed to have the form

$$\mathscr{G}(\mathbf{q}_\parallel)=\begin{cases}0, & |\mathbf{q}_\parallel|>q_{\max},\\ Cq^{-\beta}, & q_{\max}\geqslant|\mathbf{q}_\parallel|\geqslant q_{\min},\\ 0, & q_{\min}>|\mathbf{q}_\parallel|.\end{cases} \tag{2.4}$$

Under the assumptions $X^N\equiv\mathbf{R}^3$, the system scale is unbounded and $\mathscr{G}$ has the form, $\mathscr{G}(\mathbf{q}_\parallel)=\text{const}\times|\mathbf{q}_\parallel|^{-\beta}$, Pfeiffer[5] has shown that the Hausdorf dimension of the surface is given by

$$D_H=\max[2,\tfrac{1}{2}(7-\beta)]. \tag{2.5}$$

This is important because it provides the connection between the work presented in this paper and the popular fractal concept. It must be stressed here that this dimension is the Hausdorf dimension and *not* the Euclidian dimension. The two only coincide when $D_H\in Z$, otherwise it does not have a very good physical interpretation as a physical dimension. The only real meaning that can be attached to the Hausdorf dimension is that the surface is self-similar and scales as $(\text{const})^\beta$.

III. PERTURBATIVE TECHNIQUES

There is a great difference between perturbing the shape of the surface upon which a boundary condition is made, and perturbing the potential of the Hamiltonian. Of course, one can always express the boundary conditions in such a way that they add to the potential in some natural way. For the case of a boundary between two different media this would be done by the addition of terms proportional to $\theta(z-h(\mathbf{x}))$, to the potential. This requirement will produce a mathematical nightmare when one actually tries to calculate interesting quantities, since any mathematical treatment of the theta function will contain singularities in its derivatives. This constraint forces one to work with perturbations that are well behaved.

After adding these terms to the potential, the procedure continues with finding the Green's function and ends with the method of successive approximation. But, the Green's function must satisfy the boundary conditions on the perturbed surface, as well as the Hamiltonian equation. For a rough surface there is no hope of finding a Green's function that satisfies the boundary conditions exactly. Thus, one must use the method of successive approximation on the Green's function as well. It is here that one runs into difficulty, because solving the necessary integral equation produces a logarithmically divergent series.[6] The Green's function method tacitly assumes that the integral over the boundary is well defined when, in fact, the power law behavior assumed for rough surface covariance, produces singular solutions as the boundary conditions approach Dirichlet boundary conditions. Abandoning this approach will require a direct construction of the the perturbed solution. It is unclear as to whether this approach can be extended to all systems of PDEs with "rough" boundaries, but it is expected that in principle one could carry out this procedure on any separable system.

Let the system under consideration be

$$\mathbf{H}\Psi=E\Psi, \quad \Psi(\mathbf{x}) \text{ some field, and } \mathbf{x}\in X^N, \tag{3.1a}$$

and satisfy the boundary conditions

$$\left[\frac{\partial\Psi}{\partial n}+f_0\Psi\right]_{\text{on } S}=g_0(S),\quad S \text{ as given from Definition 1,} \tag{3.1b}$$

with normal derivative

$$\frac{\partial}{\partial n}=-\epsilon g_{\|}^{\mu\nu}\frac{\partial h}{\partial x^{\mu}}\frac{\partial}{\partial x^{\nu}}+(1+\epsilon^2\,\partial_{\mu}h\,\partial^{\mu}h)^{-1/2}\frac{\partial}{\partial x_{\perp}}. \tag{3.1c}$$

Further suppose Ψ and E can be represented as a power series in ϵ, where ϵ is given as some small parameter determining the surface height in Definition 1:

$$\Psi=\sum_{n=0}^{\infty}\epsilon^n\Psi_n\approx\Psi_0+\epsilon\Psi_1+\epsilon^2\Psi_2+\mathcal{O}(\epsilon^3),$$
$$E=\sum_{n=0}^{\infty}\epsilon^nE_n\approx E_0+\epsilon E_1+\epsilon^2E_2+\mathcal{O}(\epsilon^3), \tag{3.2}$$

where Ψ_0 is known to satisfy

$$\mathbf{H}\Psi_0=E_0\Psi_0 \text{ and } \left[\frac{\partial\Psi_0}{\partial x_{\perp}}+f_0\Psi_0\right]_{\text{on } S_0}=g_0(S_0). \tag{3.3}$$

Then (3.1b) is expanded about $x_{\perp}=0$ in a Taylor series, and equating powers of ϵ produces perturbed boundary conditions. The solutions Ψ_1, Ψ_2, E_1, and E_2 define a new boundary condition defined as

$$\left[\left\langle\frac{\partial\Psi}{\partial n_0}\right\rangle+f(S_0)\langle\Psi\rangle\right]_{\text{on } S_0}=g(S_0). \tag{3.4}$$

Where the averages are to be performed as outlined in Sec. II.

For the semiinfinite case with $g(S)=0$ in (3.1b) f will be given by the ratio,

$$-\left\langle\left.\frac{\partial\Psi}{\partial n}\right|_{\text{on } S_0}\right\rangle(\langle\Psi|_{\text{on } S_0}\rangle)^{-1}\equiv f(S_0). \tag{3.5}$$

Under our averaging procedure, all first-order dependency vanishes. So,

$$f\approx f_0-\epsilon^2\left(\frac{\langle(\partial\Psi_2/\partial x_{\perp})(S_0)\rangle}{\Psi_0(S_0)}-f_0\frac{\langle\Psi_2(S_0)\rangle}{\Psi_0(S_0)}\right). \tag{3.6}$$

The solutions (3.4) are valid anywhere inside X^N, and not just inside the perturbed surface S, which we consider the physical surface. If one views (3.1b) as a constraint equation, then (3.4) will satisfy some other set of boundary conditions on S_0. Here, f as calculated in (3.6) is that f, such that the average fields obey (3.1b) at S. It should be valid to assume the rhs of (3.6) should contain powers of $\epsilon h(x_{\|})$, since the perturbed solutions are constrained by S. In this dependence $\mathcal{G}(\mathbf{q}_{\|})$ occurs naturaly, and thus (3.6) will have dependency upon the interval $(q_{\min},q_{\max})$. The behavior of f under the transformation of $q\to q_{\min}+\delta q_{\min}$ is then a renormalization of f, and its flow governed by the renormalization group equation (RGE) found by differentiating (3.6) with respect to $q_{\min}$. Physically this says, that given some strength for f at the microscopic level ($f_{\text{micro}}(q=q_{\max})$), we may find a macroscopic strength by following the one-parameter family of solutions created by the ODE, for f, to the limit $q=q_{\min}$, which is our infrared cutoff of the Fourier transformed surface. It should not be surprising that $f\propto f_0(A'/A)+\zeta(S)$ where A' is the area of the perturbed surface. It turns out that there is also a nonlinear term ζ, in the RGE.

Technically (3.6) could be used to obtain the RGE for a set of closed systems. But, it will not prove easy or sometimes possible to find a second-order eigenfunction with good convergence properties. Again, this is exemplified for Dirichlet boundary conditions ($f_0\to\infty$), as is discussed at length in Ref. 6. On the other hand, one can find a second-order expansion for the eigenvalue that converges absolutely.

It will prove beneficial to rewrite E in (3.2) in terms of a new variable k^2. This will allow us to cast the system of equations (3.1) into wave equation format, and develop a variational principle. Let

$$k^2=\sum_{n=0}^{\infty}\epsilon^nk_n'^2\approx k_0'^2+\epsilon k_1'^2+\epsilon^2k_2'^2+\mathcal{O}(\epsilon^3), \tag{3.7}$$

or using the binomial expansion we identify k_n with the coefficient of ϵ^n, and so on,

$$k\approx k_0+\epsilon\frac{1}{2}\frac{k_1^2}{k_0}+\epsilon^2\left(\frac{1}{2}\frac{k_2^2}{k_0}-\frac{1}{8}\frac{k_1^4}{k_0^3}\right)+\mathcal{O}(\epsilon^3). \tag{3.8}$$

After finding the perturbed eigenvalue k, let $k_0\to k$ in Ψ_0 and use

$$\left[\frac{\partial\Psi_0}{\partial x_{\perp}}+f\Psi_0\right]_{\text{on } S_0}=g(S_0) \tag{3.9a}$$

to define the renormalized value of f. Here, (3.9a) will produce an eigenvalue equation that will in general be transcendental. If $\mathbf{H}$ is ∂^2, for example, in the case of X^N being an N-dimensional box

$$k\tan(kL')=f. \tag{3.9b}$$

Or in the case of $X^N\cong S_a^N$ (the N-dimensional sphere of radius a),

$$-\frac{j_n'(ka)}{j_n(ka)}=\frac{f}{k}, \tag{3.10}$$

where the j_n's are spherical bessel functions.

Now we expand (3.9b) or (3.10) in a power series in ϵ and equate terms with the ϵ expansion of f, this will define a change in f and thus the RGE can be defined in the same manner as above. For (3.9b) this will be

$$\begin{aligned}f_0&=k_0\tan(k_0L'),\\ f_1&=(k_1/k_0)(f_0+L'(f_0^2+k_0^2)),\\ f_2&=(k_2/k_0)(f_0+L'(f_0^2+k_0^2))\\ &\quad+(k_1^2/k_0^2)L'((f_0^2+k_0^2)(1+f_0)),\end{aligned} \tag{3.11}$$

and for (3.9b)

$$
\begin{aligned}
f_0 &= (1/a) - k_0 \cot(k_0 a) \\
f_1 &= (k_1/k_0)(a(f_0^2 + k_0^2) - f_0) \\
f_2 &= (k_2/k_0)(a(f_0^2 + k_0^2) - f_0) \\
&\quad + j_0^{-2}(k_0 a) f_0 (k_1^2/k_0^2),
\end{aligned} \tag{3.12}
$$

where averages may now be taken to find the average values of both f_1 and f_2. The averaging procedure will then relate the surface structure to some new value of f, and a RGE similar to (3.6) is then derived.

IV. THE SEMIINFINITE SPACE

An interesting problem of moderate difficulty is a wave impinging upon a random surface in a semiinfinite medium. An example would be that of an electromagnetic wave reflecting from a rough dielectric. To simplify the problem and determine where an analysis of this problem might lead, a linear approximation is first calculated. Close to the surface there is no reason to believe that it would fail. In fact, the linear approximation turns out to have the same characteristics as more complicated situations, in the sense that the main goal is to find an effective theory with renormalized parameters.

Consider the N-dimensional Laplace's equation with an arbitrary metric $g^{\mu\nu}$,

$$
g^{\mu\nu} \frac{\partial^2 \psi}{\partial x^\mu \, \partial x^\nu} = \partial^2 \psi = 0 \tag{4.1}
$$

[i.e., $\mathbf{H} = \partial^2$ in (3.1a)], and boundary conditions (3.1b) with $g_0(S) = 0$. For the diffusion equation our boundary conditions, with D the diffusion constant of the fluid, and ρ some surface interaction, would modify (3.1b) to

$$
D(n_\mu \, \partial^\mu \psi)|_{\text{on } S} + \rho \psi|_{\text{on } S} = 0 \text{(Ref. 3)}, \tag{4.2}
$$

where n_μ are just the components of the unit normal pointing out of the semiinfinite volume that our solution exists. We still use the more compact notation of (3.1b) with $g(S) = 0$.

Under the linear approximation it is most easy to write down the form of the expected solutions, and the boundary conditions to $\mathcal{O}(\epsilon^2)$:

$$
\begin{aligned}
\psi_0(\mathbf{x}) &= \alpha + \gamma x_\perp, \\
\psi_1(\mathbf{x}) &= \int d^{N-1}\mathbf{k}_1 \, e^{-i\mathbf{k}_1 \cdot \mathbf{x}_\parallel - k_1 x_\perp} \tilde{\psi}_1(\mathbf{k}_1), \\
\psi_2(\mathbf{x}) &= \int d^{N-1}\mathbf{k}_2 \, e^{-i\mathbf{k}_2 \cdot \mathbf{x}_\parallel - k_2 x_\perp} \tilde{\psi}_2(\mathbf{k}_2).
\end{aligned} \tag{4.3}
$$

Where $k_2 = |\mathbf{k}_{2\parallel}|$, $k_2 = |\mathbf{k}_{2\parallel}|$, and integration over k_1 has been carried out with the requirement that the perturbed solutions be finite at infinity. The boundary conditions are

$$
\mathcal{O}(\epsilon^0): \left[\frac{\partial \psi_0}{\partial x_\perp}\right]_{x\perp = 0} = [f_0 \psi_0]_{x_\perp = 0},
$$

$$
\mathcal{O}(\epsilon^1): \left[h \frac{\partial^2 \psi_0}{\partial x_\perp^2} + \frac{\partial \psi_1}{\partial x_\perp}\right]_{x_\perp = 0} = \left[f_0 \psi_1 + f_0 h \frac{\partial \psi_0}{\partial x_\perp}\right]_{x_\perp = 0},
$$

$$
\mathcal{O}(\epsilon^2): \left[\frac{\partial \psi_2}{\partial x_\perp} + h \frac{\partial^2 \psi_1}{\partial x_\perp^2} - g_\parallel^{\mu\nu} \frac{\partial h}{\partial x^\mu} \frac{\partial \psi_1}{\partial x^\nu} - \frac{\partial^\nu h \, \partial_\nu h}{2} \frac{\partial \psi_0}{\partial x_\perp}\right]_{x_\perp = 0} = \left[f_0 \psi_2 + f_0 h \frac{\partial \psi_1}{\partial x_\perp}\right]_{x_\perp = 0}. \tag{4.4}
$$

Omitting the tedious algebra, the solutions to (4.3) and (4.4) are

$$
\tilde{\psi}_1(\mathbf{k}_1) = -f_0 \gamma \tilde{h}(\mathbf{k}_1)/(k_1 + f_0) \tag{4.5a}
$$

and

$$
\begin{aligned}
\tilde{\psi}_2(\mathbf{k}_2) = \frac{\gamma}{f_0 + k_2} \int d^{N-1}\mathbf{k}_1 \, \tilde{h}(\mathbf{k}_1) \tilde{h}(\mathbf{k}_2 - \mathbf{k}_1) \\
\times \left[\frac{g_\parallel^{\mu\nu} k_{1\mu} (k_{2\nu} - k_{1\nu})}{2} \right. \\
\left. - \frac{f_0 g_\parallel^{\mu\nu} k_{1\mu} k_{2\nu}}{f_0 + k_1} - \frac{f_0^2 k_1}{f_0 + k_1}\right].
\end{aligned} \tag{4.5b}
$$

The average process in Sec. II is applied to find the average field $\langle \psi_1 \rangle = 0$, so

$$
\begin{aligned}
\langle \psi \rangle &\approx \psi_0 + \epsilon^2 \langle \psi_2 \rangle \\
&= \alpha + \gamma x_\perp - \epsilon^2 \alpha \int d^{N-1}\mathbf{k} \left[\frac{k^2}{2} + \frac{f_0^2 k}{f_0 + k}\right] \mathcal{G}(\mathbf{k}).
\end{aligned} \tag{4.6}
$$

It would be tempting to use $f = (\partial\psi/\partial n)/\psi$ as the definition of f so that the average would be given by $\langle f \rangle = \langle (\partial\psi/\partial n)/\psi \rangle$. As pointed out in Sec. III though, there is no reason *a priori* not to select this renormalization scheme. But, Secs. III and V, show that there is only one allowable scheme for the closed system. The closed systems under investigation can be continuously enlarged to the limit of the semiinfinite case. Thus, under these conditions, choice of the scheme that produces the correct limiting behavior is forced upon us. This choice does not include the squares of the first-order term nor any of its derivatives, implying that the correct choice is $f = \langle \partial\psi/\partial n \rangle / \langle \psi \rangle$, (3.6), which yields,

$$
f \approx \frac{\gamma}{\alpha} \left\{1 + \epsilon^2 \int d^{N-1}\mathbf{k} \left[\frac{k^2}{2} + \frac{f_0^2 k}{f_0 + k}\right] \mathcal{G}(\mathbf{k})\right\}. \tag{4.7}
$$

Using (2.4) and explicitly writing out each step

$$
\begin{aligned}
f \approx f_0 \{1 + \epsilon^2 A S^{N-1} C \\
\times \int_{q_{\min}}^{q_{\max}} dk \, k^{N-2-\beta} \left[\frac{k^2}{2} + \frac{f_0^2 k}{f_0 + k}\right]\}.
\end{aligned} \tag{4.8}
$$

Here, $A S^{N-1}$ is the surface area of a unit $N-1$ sphere,

$$
A S^{N-1} = \frac{2\pi}{\Gamma(N/2)}.
$$

Absorb the $A S^{N-1}$ into the definition of q and f, differentiate (4.8) with respect to $q_{\min}$, drop the (min) subscript, and substitute in f to $\mathcal{O}(\epsilon^2)$ for f_0. Then, the RGE is given by

$$
\frac{df}{dq} \approx -\epsilon^2 f q^{1-\beta} \left[\frac{q^2}{2} + \frac{f^2 q}{f+q}\right]. \tag{4.9}
$$

A more complicated situation is that of a plane-wave

incident on a boundary constructed as before, but without a linear approximation. Here, terms occur in the RGE for f that are proportional to the new area and terms that are nonlinear in nature, including some that depend on the surface structure through gradients and scalar products. Thus the particular renormalization is not unique and will depend on the spatial characteristics of the incoming wave. No longer a static problem, the Helmholtz equation is solved

$$\partial^2\psi + k^2\psi = 0. \tag{4.10}$$

The solutions are expected to take the form

$$\psi_0(\mathbf{x}) = e^{-i\mathbf{k}\cdot\mathbf{x}} + \mathscr{R}_0 e^{+i\mathbf{k}'\cdot\mathbf{x}},$$

$$\psi_1(\mathbf{x}) = \int d^N\mathbf{k}_1 e^{-i\mathbf{k}_1\cdot\mathbf{x}}\tilde{\psi}_1(\mathbf{k}_1),$$

$$\psi_2(\mathbf{x}) = \int d^N\mathbf{k}_2 e^{-i\mathbf{k}_2\cdot\mathbf{x}}\tilde{\psi}_2(\mathbf{k}_2). \tag{4.11}$$

To second order we not only have to worry about derivatives of higher order but the concept of a new area enters the problem. Our boundary conditions are, to second order

$$\mathscr{O}(\epsilon^0):\left[\frac{\partial\psi_0}{\partial x_\perp}\right]_{x_\perp=0} = [f_0\psi_0]_{x_\perp=0},$$

$$\mathscr{O}(\epsilon^1):\left[-\frac{\partial\psi_1}{\partial x_\perp} + f_0\psi_1\right]_{x_\perp=0}$$
$$= \left[h\frac{\partial^2\psi_0}{\partial x_\perp{}^2} - g_\parallel^{\mu\nu}\frac{\partial h}{\partial x^\mu}\frac{\partial\psi_0}{\partial x^\nu} - f_0 h\frac{\partial\psi_0}{\partial x_\perp}\right]_{x_\perp=0}, \tag{4.12}$$

$$\mathscr{O}(\epsilon^2):\left[-\frac{\partial\psi_2}{\partial x_\perp} + f_0\psi_2\right]_{x_\perp=0}$$
$$= \left[-\left(g_\parallel^{\mu\nu}\frac{\partial\psi_1}{\partial x^\mu}\frac{\partial h}{\partial x^\nu} - h\frac{\partial^2\psi_1}{\partial x_\perp{}^2} + f_0 h\frac{\partial\psi_1}{\partial x_\perp}\right)\right.$$
$$-\left(g_\parallel^{\mu\nu}h\frac{\partial h}{\partial x^\mu}\frac{\partial^2\psi_0}{\partial x^\nu\partial x_\perp} + \frac{\partial_\mu h\,\partial^\mu h}{2}\frac{\partial\psi_0}{\partial x_\perp}\right.$$
$$\left.\left.-\frac{h^2}{2}\frac{\partial^3\psi_0}{\partial x_\perp{}^3} + \frac{f_0 h^2}{2}\frac{\partial^2\psi_0}{\partial x_\perp{}^2}\right)\right]_{x_\perp=0}.$$

The $\mathscr{O}(\epsilon^0)$ boundary conditions require $\mathscr{R}_0$ to be given by

$$\mathscr{R}_0 = -(f_0 + ik_\perp)/(f_0 - ik_\perp), \tag{4.13}$$

while continuity at the boundary implies $\mathbf{k}_\parallel = -\mathbf{k}'_\parallel$ and $k_\perp = k_\perp{}'$, which is contained within the familiar Snell's law of specular reflection. Once again we omit the edifying algebra, and obtain

$$\tilde{\psi}_1(\mathbf{k}_1) = \delta((k^2 - |\mathbf{k}_{1\parallel}|^2)^{1/2} + k_{1\perp})(\tilde{h}(\mathbf{k}_{1\parallel} - \mathbf{k}_\parallel)/(ik_{1\perp} + f_0))((\mathbf{k}_{1\parallel} - \mathbf{k}_\parallel)\cdot\mathbf{k}_\parallel(1 + \mathscr{R}_0)$$
$$+ f_0 ik_\perp(1 - \mathscr{R}_0) - k_1^2(1 + \mathscr{R}_0)),$$

$$\tilde{\psi}_2(\mathbf{k}_2) = \frac{1}{ik_{2\perp} + f_0}\int d^{N-1}\mathbf{q}\{\tilde{h}(\mathbf{k}_{2\parallel} - \mathbf{q}_\parallel)\tilde{\psi}_1(\mathbf{q}_\parallel, -(k^2 - |\mathbf{q}_\parallel|^2)^{1/2})((\mathbf{k}_{2\parallel} - \mathbf{q}_\parallel)\cdot\mathbf{q}_\parallel - k^2 + |\mathbf{q}_\parallel|^2$$
$$- if_0(k^2 - |\mathbf{q}_\parallel|^2)^{1/2}) + (\tfrac{1}{2}\mathbf{q}_\parallel\cdot(\mathbf{k}_{2\parallel} - \mathbf{q}_\parallel - \mathbf{k}_\parallel)(ik_\perp)(\mathscr{R}_0 - 1) - (ik_1^3/2)(\mathscr{R}_0 - 1)$$
$$+ \mathbf{q}_\parallel\cdot\mathbf{k}_\parallel(ik_\perp)(\mathscr{R}_0 - 1) + (f_0 k_1^2/2)(\mathscr{R}_0 + 1))\tilde{h}(\mathbf{q}_\parallel)\tilde{h}(\mathbf{k}_{2\parallel} - \mathbf{q}_\parallel - \mathbf{k}_\parallel)\}. \tag{4.14}$$

We are guided by the previous exercise in applying the averaging procedure of Sec. II to these solutions. As in (4.6) $\langle\psi\rangle \approx \psi_0 + \epsilon^2\langle\psi_2\rangle$, but from a physical standpoint $\langle\psi_2\rangle$ should propagate in the $\mathbf{k}'$ direction, because the boundary has a random structure and the average is over all possible random surfaces. This produces a spherically symmetric probability distribution of reflection directions, centered at $\mathbf{k}'$. Here, $\langle\psi_2\rangle$ should then only modify $\mathscr{R}_0$ to $\langle\mathscr{R}\rangle$ and have the correct sign such that $\langle\mathscr{R}\rangle \leqslant \mathscr{R}_0$, signifying that much of the reflected wave is scattered over other directions. So,

$$\langle\psi\rangle = \psi_0 + \epsilon^2\langle\psi_2\rangle$$
$$= e^{-i\mathbf{k}\cdot\mathbf{x}} + \langle\mathscr{R}\rangle e^{i\mathbf{k}'\cdot\mathbf{x}}$$
$$= e^{-i\mathbf{k}\cdot\mathbf{x}} + e^{i\mathbf{k}'\cdot\mathbf{x}}\left[\mathscr{R}_0 + \frac{2f_0 ik_\perp\epsilon^2}{(f_0 - ik_\perp)^2}\int d^{N-1}\mathbf{q}\left\{\frac{|\mathbf{q}_\parallel|^2}{2}\right.\right.$$
$$\left.\left. + \frac{(-k^4 + f_0k^2(iq_\perp - f_0) + iq_\perp f_0^3) + (\mathbf{q}_\parallel\cdot\mathbf{k}_\parallel)^2}{f_0(iq_\perp + f_0)}\right]\mathscr{G}(\mathbf{q})\right\}. \tag{4.15}$$

Where $q_\perp = -(k^2 - |\mathbf{q}_\parallel|^2)^{1/2}$ so that for $k < |\mathbf{q}_\parallel|$, $q_\perp = -i|q_\perp|$ and the fact that $\mathscr{G}(\mathbf{q})$ is an even function of $\mathbf{q}$ has been used to eliminate terms linear in $\mathbf{q}_\parallel$. Invoking (3.6) as before

$$\frac{df}{dq_{\min}} = \epsilon^2 f_0\frac{d}{dq_{\min}}\int d^{N-1}\mathbf{q}\left\{\frac{|\mathbf{q}_\parallel|^2}{2} + \frac{iq_\perp f_0^2}{iq_\perp + f_0} + \frac{(-k^4 + f_0k^2(iq_\perp - f_0) + (\mathbf{q}_\parallel\cdot\mathbf{k}_\parallel)^2}{f_0(iq_\perp + f_0)}\right\}\mathscr{G}(\mathbf{q}). \tag{4.16}$$

The first and second terms on the rhs are exactly what comes from the linear approximation, and the last term is what is required by the plane wave, and approaches 0 as $k \to 0$ (the linear approximation limit).

V. THE CLOSED SYSTEM

Applying the same procedure worked out in Secs. III and IV to that of a closed system is an important exercise, since the ideas of a particle in a box described by a scalar field

are prevalent throughout much of the literature. One of the difficulties that will arise is that control over $\mathbf{k}_0$ is lost. Instead of $\mathbf{k}_0$ remaining constant, a new mode is created, that is a function of all modes of the unperturbed problem, the surface shape, and hence the Fourier components of the surface.

In terms of energy, one expects the first-order shift to be proportional to $h_{0,0}$, the constant Fourier component of the surface, with sign such that an increase in volume produces a decrease in energy. On the other hand, the second-order shift is expected to behave as some multiple of the new area. But as Sec. IV has shown, one should also expect nonlinear terms to appear as well.

As pointed out in Sec. III, one ought to be careful with the process of renormalizing f_0. It should be obvious that if f_0 were to be treated as some continuous parameter, $f_0 \in [0, \infty)$, then the limit $\to 0$ is the von Neumann boundary condition limit, and $f_0 \to \infty$ is the Dirichlet boundary limit. In terms of the energy spectrum, the ground state is $E_0 = 0$ for $f_0 = 0$ and $E_0 = \pi\hbar c/2L$ at $f_0 = \infty$. The point is that $f_0 = 0$ is identical to a soft boundary that absorbs all incident waves, so that it is not surprising that $E_0 = 0$.

For the first calculation, let X^N be the N-dimensional hypercube with volume $L^{N-1}L'$, where the length L' is taken in the perpendicular direction. The second calculation will use the sphere S^N, with radius a. To make the proper connection with the work in Sec. IV, let the transverse scales become very large compared to the perpendicular direction, then let the perpendicular direction become large as well.

We return to Helmholtz's equation:

$$\partial^2\psi + k^2\psi = 0,$$

with

$$n_\mu \partial^\mu \psi|_{\text{on } S} + f_0 \psi|_{\text{on } S} = g(S)$$

($\hat{\mathbf{n}}$ points out of the boundary) while the normal derivative is zero on the transverse boundaries,

$$\frac{\partial\psi}{\partial n}(x_1 = 0, L, \ldots, x_{N-1} = 0, L) = 0 \tag{5.1}$$

and

$$\frac{\partial\psi}{\partial n}(x_N = 0) = 0,$$

x_N will be represented as $x_\perp$. Labeling a particular solution ψ as $\psi_{n_1,\ldots,n_N}$, a typical solution of the system of equations (3.1a)–(3.1c) for the unperturbed problem will have the form

$$\psi_{n_1,\ldots,n_N} = C_{n_1,\ldots,n_N} \cos(k_{n_1}x_1)\cos(k_{n_2}x_2) \cdots \cos(k_{n_{N-1}}x_{N-1})\cos(k_{n_N}x_\perp), \tag{5.2a}$$

where the $C_{n_1,\ldots,n_N}$ are the normalization constants defined as

$$C^{-2}_{n_1,\ldots,n_N} = \left(\frac{L}{2}\right)^{N-1}\left(\frac{L'}{2} + \frac{1}{4k_{n_N}}\sin(2k_{n_N})\right)\prod_{i=1}^{N-1} 2^{\delta_{on_i}} \tag{5.2b}$$

and the boundary conditions yield

$$\tan(k_{n_N}L') = f_0/k_{n_N}, \tag{5.3a}$$

$$k_{n_i} = n_i\pi/L, \quad i \neq N, \tag{5.3b}$$

$$k^2 = k^2_{n_1} + \cdots + k^2_{n_N}. \tag{5.3c}$$

To simplify the calculations as far as possible, let $N = 3$, change the notation to $n_1 = n$, $n_2 = l$, $n_3 = m$ with $l = n = 0$ and $m = 1$. Since we will be working in a finite domain, the Fourier integrals of Sec IV will become Fourier series. Lastly, the results of Appendix A may be used, and thus only the first-order corrections need be constructed directly. The rest being given by a variational principle (A5). So,

$$h(\mathbf{x}) = \sum_{n,l=-\infty}^{+\infty} e^{i\mathbf{k}_{n,l}\cdot\mathbf{x}} h_{n,l} \tag{5.4}$$

and

$$\psi_1(\mathbf{x}) = \sum_{n,l=-\infty}^{+\infty} e^{i\mathbf{k}_{n,l}\cdot\mathbf{x}} \tilde{\psi}_{n,l}(x_\perp), \tag{5.5}$$

with

$$\mathbf{k}_{n,l} = (n\pi/L)\hat{\mathbf{x}} + (l\pi/L)\hat{\mathbf{y}}.$$

Equations (3.1a)–(3.1c) to $\mathcal{O}(\epsilon)$ are

$$\partial^2(\psi_0 + \epsilon\psi_1) + k_0^2\psi_0 + \epsilon k_1^2\psi_0 + \epsilon k_0^2\psi_1 = 0, \tag{5.6a}$$

$$\left[\frac{\partial}{\partial n}(\psi_0 + \epsilon\psi_1) + f_0(\psi_0 + \epsilon\psi_1)\right]_{S_0+S_1} = 0. \tag{5.6b}$$

The notation $|_{S_0+S_1}$ means to evaluate on the perturbed surface to first order, using our formula for $\partial/\partial n$ and expanding about $x_\perp$ in powers of $h(\mathbf{x})$:

$$\frac{\partial}{\partial n} \approx \frac{\partial}{\partial x_\perp} - \epsilon g^{\mu\nu}_{\parallel}\frac{\partial h}{\partial x^\mu}\frac{\partial}{\partial x^\nu}. \tag{5.6c}$$

Solving for ψ_1 with the assumption

$$\psi_0 = C_0\cos(k_0 x_\perp),$$

with

$$\psi_0(L') = C_0^2\cos^2(k_0L') = \frac{2}{L^2}\frac{k_0^2}{f_0 + L'(k_0^2 + f_0^2)} \tag{5.7}$$

we find

$$\tilde{\psi}_{n,l}(x_\perp) = \begin{cases} -C_0\dfrac{k_1^2}{2k_0}x_\perp\sin(k_0x_\perp), & n = l = 0; \\ -\dfrac{C_0h_{n,l}(k_0^2 + f_0^2)\cos(k_0L')}{[k_0^2 - k_{n,l}^2]^{1/2}\sin([k_0^2 - k_{n,l}^2]^{1/2}L') - f_0\cos([k_0^2 - k_{n,l}^2]^{1/2}L')}\cos([k_0^2 - k_{n,l}^2]^{1/2}x_\perp), & \text{otherwise} \end{cases} \tag{5.8a}$$

and

$$k_1^2 = -\frac{2k_0^2(f_0^2+k_0^2)h_{0,0}}{f_0+k_0^2L'+f_0k_0L'}. \tag{5.8b}$$

Now, before invoking the variational principle worked out in Appendix A,

$$[k^2] = k_0^2 + k_1^2 - \epsilon^2 k_1^2 \int dV \psi_0\psi_1 + \int dS\, \psi_0\left(\frac{\partial}{\partial n}+f_0\right)(\psi_0+\psi_1), \tag{5.9}$$

we note two facts that simplify our calculation. Fact 1: $(\partial/\partial n + f_0)(\psi_0+\psi_1)$ is a second-order term by difinition. Fact 2: All terms with one or two $h_{0,0}$ in them will average to zero by (2.3). So, any term with k_1 averages to zero. Thus Facts 1 and 2, (2.3), (3.8), and (3.11) give

$$\langle f_2\rangle = \sum_{(n,l)\neq(0,0)} \left\{ \frac{k_0^2\cos([k_0^2-k_{n,l}^2]^{1/2}L') + f_0[k_0^2-k_{n,l}^2]^{1/2}\sin([k_0^2-k_{n,l}^2]^{1/2}L')}{[k_0^2-k_{n,l}^2]^{1/2}\sin([k_0^2-k_{n,l}^2]^{1/2}L') - f_0\cos([k_0^2-k_{n,l}^2]^{1/2}L')}(k_0^2+f_0^2) + \frac{f_0k_{n,l}^2}{2}\right\}\mathscr{G}_{n,l}. \tag{5.10}$$

There is an obvious resemblance between this and the case of reflection from a rough surface in a semiinfinite medium, worked out in Sec. IV. Letting $\mathbf{k} = k\hat{\mathbf{z}}$, and $k \ll f_0 \ll k_{n,l}$ implies

$$\langle f_2\rangle \approx \sum_{(n,l)\neq(0,0)} \left\{\frac{f_0k_{n,l}^2}{2} + \frac{f_0^3k_{n,l}}{f_0+k_{n,l}}\right\}\mathscr{G}_{n,l}, \tag{5.11}$$

which is in exact agreement with (4.9), showing that the linear approximation is reasonable.

For the case of the sphere, the unperturbed wave function is taken as

$$\psi_0 = C_0 j_0(k_0r) = C_0(\sin k_0r/k_0r), \tag{5.12a}$$

$$C_0 = (2/a^3)^{1/2}j_0^{-1}(k_0a)[k_0/(k_0-f_0)], \tag{5.12b}$$

where $j(k_0r)$ is the spherical Bessel function of the first kind. And the boundary conditions are (3.1c), with explicit representation of $\partial/\partial n$ being given by

$$\frac{\partial}{\partial n} \approx \left(1-\frac{\epsilon^2}{2}\partial_\mu h\,\partial^\mu h\right)\frac{\partial}{\partial r} - \frac{1}{a^2}\frac{\partial h}{\partial\theta}\frac{\partial}{\partial\theta} - \frac{1}{a^2\sin^2\theta}\frac{\partial h}{\partial\phi}\frac{\partial}{\partial\phi}. \tag{5.13}$$

Applying the same procedure as above with the boundary now expressed in terms of spherical harmonics

$$h(x) = \sum_{l,m} h_{l,m}Y_l^m(\theta,\phi), \tag{5.14}$$

we find:

$$\psi_1 = C_{1,0}\cos(k_0r) + \sum_{l,m} C_{1,l,m}Y_l^m(\theta,\phi)j_l(k_0r). \tag{5.15}$$

Here, $Y_l^m(\theta,\phi)$ is the spherical harmonic, with phase convention from Arfkin.[7] It is then straightforward to calculate the perturbed eigenvalue to $\mathcal{O}(\epsilon)$ and the constants $C_{1,0}$ and $C_{1,l,m}$:

$$k_1^2 = k_0^2\frac{C_{1,0}}{2C_0} = -\frac{2k_0h_{0,0}}{a}\frac{f_0^2+k_0^2-(2f_0/a)}{f_0^2+k_0^2-(f_0/a)}, \tag{5.16a}$$

$$C_{1,0} = -\frac{C_0h_{0,0}}{a}\frac{f_0^2+k_0^2-(2f_0/a)}{f_0^2+k_0^2-(f_0/a)}, \tag{5.16b}$$

$$C_{1,l,m} = \frac{(f_0^2+k_0^2-2f_0/a)C_0h_{l,m}}{[\partial j_{f(k_0a)/\partial a}+f_0j_l](k_0a)} = C'_{1,l}h_{l,m}. \tag{5.16c}$$

Following the same procedure that led to (5.10) leads to

$$\langle f_2\rangle = \frac{a(f_0^2+k_0^2)-f_0}{a^2(k_0-f_0)^2}\left\{\left[\frac{1}{2}\left(f_0^2+2k_0^2-\frac{6f_0}{a}\right)\sum_l(2l+1)\mathscr{G}'(l)\right]\right.$$
$$\left. + a\left(f_0^2+k_0^2-\frac{2f_0}{a}\right)\sum_l\left[\left(f_0\frac{\partial_{j_l}(k_0a)}{\partial a}+\frac{\partial^2{}_{j_l}(k_0a)}{\partial a^2}\right)\left(\frac{\partial_{j_l}(k_0a)}{\partial a}+f_{0j_l}(k_0a)\right)^{-1}\right](2l+1)\mathscr{G}'(l)\right.$$

$$+\left[\frac{1}{4\pi a}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\mathscr{G}'(l)\left(\frac{f_0}{2}-\frac{j_l(k_0a)}{j_0(k_0a)}\left[\left(f_0^2+k_0^2-\frac{2f_0}{a}\right)\left(\frac{\partial_{j_l}(k_0a)}{\partial a}+f_{0j_l}(k_0a)\right)^{-1}\right]\right)\int d\Omega\left(\frac{\partial Y_l^m}{\partial\theta}\frac{\partial Y_l^{*m}}{\partial\theta}\right.\right.$$

$$\left.\left.+\frac{1}{\sin^2\theta}\frac{\partial Y_l^m}{\partial\phi}\frac{\partial Y_l^{*m}}{\partial\phi}\right)\right]\right\}. \tag{5.17}$$

It is much more difficult to get at the meaning of (5.17) due to the complex nature of the distribution function $\mathscr{G}'(l)$. But the same term involving the new area of the perturbed surface is present. As well, the second summation is expected to yield the term f_0^3, since it is exactly this term in the variational equation (A5) that leads to this term in (5.10). The interesting point that needs to be made about (5.17) is that it appears possible to have a fixed point in the renormalization of f. Namely, there seems to be no reason why $\langle f_2\rangle = 0$ is not a possibility, unlike (4.9) and (5.11). The implication is that under the right circumstances $f_0 \to f_{fp}$, the fixed point, regardless of the extent to which the surface is fractal-like, and thus the cutoff can be removed from the theory. Unfortunately, this is all that can be said about (5.17), because a fully detailed analysis is still forthcoming, and will be the subject of the next paper.

VI. CONCLUSION

Under a vast set of conditions, (4.9) seems to be a good approximation of the RGE for f. It should be emphasized that what we have done is to solve the unperturbed problem with boundary conditions (1.2) and the constraint (1.3). The true $\langle f\rangle$ in (1.2) is in fact the measurable quantity much the same as m_{phys} and not m_0 (the bare mass) is the physically measurable mass of the electron for quantum field theory.[8]

To see the power of the philosophy of the renormalization theory, consider the problem of NMR spectroscopy on pores in sandstone as in Ref. 3. In this example, the size of a typical pore is on the order of 10^{-6} m, and no scales are probed with size $\leqslant 10^{-10}$ m. Under the assumption that the diffusion time scale is large compared to f_0 (i.e., $k_0 \ll f_0$), then the area term in (4.9) dominates at all scales except close to the lower cutoff frequency of the surface spectrum, or $\sim 10^6\,\text{m}^{-1}$. The renormalization scale factor of some f_0 is then approximated by

$$(f/f_0)|_{\beta=1.5} \sim e^{k_{\min}^{4-\beta}/2(4-\beta)} = e^{10^{15}}. \tag{6.1}$$

For any realistic f_0, f is considered to be effectively infinite, and the boundary conditions well approximated by Dirichlet conditions.

Another application of this idea is light reflecting from a mirror. Since any mirror surface can be considered rough at some scale, any field reflecting from the surface can have drastically renormalized boundary conditions if the surface roughness occurs at a high enough frequency in the power spectrum of the surface. This naturally leads to the concept of the two-scale model of wave reflection from a rough surface.[9] The two-scale model divides up the surface power spectrum into two distinct regions and tries to find suitable physical interpretation for the effect these two regions impose upon the scattering cross section. The analysis seems to explain the high-frequency region of the surface as a redefinition of the system boundary conditions.

Further investigation into the region of validity of (4.9) will require accurate numerical calculations. As of yet only preliminary efforts in this direction have been made. Although they are preliminary, these numerical calculations seem to give a smaller renormalization factor than that calculated in (6.1), but it can still be large and has not been observed to be less than 10^{30}. Subjects that may also prove interesting are the range of validity and the conditions for (5.17) to have a fixed point. As well, the question of where the solution to (4.9) does not exist and what the physical characteristics of the surface are which produce this indeterminate solution need investigation.

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APPENDIX A: DERIVATION OF EQ. (5.9)

To derive a variational principle equation for the eigenvalue in a finite volume we consider the equation we want to solve. For example, (4.10) with boundary conditions (3.1b). We start by defining a functional equation for the eigenvalue and follow the notation of Ref. 6:

$$[k^2]\int dV\,\psi^2 = -\int dV\,\psi\,\partial^2\psi + \int dS\,\psi\frac{\partial\psi}{\partial n}, \tag{A1}$$

where we have assumed that $\psi \in \mathbf{R}$ and the boundary conditions have not been specified. If we vary (A1), we find

$$\delta[k^2]\int dV\,\psi^2 + 2[k^2]\int dV\,\psi\,\delta\psi$$

$$= -2\int dV\,\delta\psi\,\partial^2\psi + \int dS\,\delta\psi\frac{\partial\psi}{\partial n}. \tag{A2}$$

So we would like to find something to add to the rhs of (A1), such that under variation, and inclusion of the exact answer $\delta[k^2] = 0$. Obviously, we add $f_0\int dS\,\psi^2$:

$$\Rightarrow [k^2] = -\int dV\,\psi\,\partial^2\psi + \int dS\,\psi\left(f_0\psi + \frac{\partial\psi}{\partial n}\right)$$

$$\times\left(\int dV\,\psi^2\right)^{-1}. \tag{A3}$$

Using the exact normalized wave function, the surface integral vanishes and

$$[k^2] \to -\int dV \psi \partial^2 \psi.$$

The next step is to expand ψ, as in (3.2), to $\mathcal{O}(\epsilon)$. Inclusion of this first-order solution into (A3) should produce the correct eigenvalue to the next highest order, or $\mathcal{O}(\epsilon^2)$. Explicily,

$$[k^2] \approx -\int dV(\psi_0 + \epsilon\psi_1)\partial^2(\psi_0 + \epsilon\psi_1) + \int dS(\psi_0 + \epsilon\psi_1)\left(f_0 + \frac{\partial}{\partial n}\right)(\psi_0 + \epsilon\psi_1) \times\left(\int dV(\psi_0 + \epsilon\psi_1)^2\right)^{-1}. \tag{A4}$$

Because $\psi_0 + \epsilon\psi_1$ satisfies the boundary conditions to first order, and ψ_0 is normalized, (A4) can be rewritten as

$$[k^2] = k_0^2 + \epsilon k_1^2 - \epsilon^2 k_1^2 \int dV \psi_1 \psi_0 + \int dS \psi_0\left(\frac{\partial}{\partial n} + f_0\right)(\psi_0 + \epsilon\psi_1). \tag{A5}$$

It should be pointed out that the integrations are carried out only over the unperturbed volume, since integration over the perturbed volume brings in only higher orders of ϵ. Thus (5.9) has been proved.

APPENDIX B: JUSTIFYING EQ. (3.5)

We will now need to justify our particular choice of renormalization scheme. We are left with an ambiguity in the definition of our renormalized f, in the semiinfinite scenario. We can choose f to satisfy either:

$$f(S') \equiv \left\langle \frac{\partial\Psi/\partial n|_{\text{on } S'}}{\Psi|_{\text{on } S'}} \right\rangle \tag{B1}$$

or

$$f(S') \equiv \frac{\langle \partial\Psi/\partial n|_{\text{on } S'} \rangle}{\langle \Psi|_{\text{on } S'} \rangle}. \tag{B2}$$

There is no reason *a priori* to choose (B1) over (B2). But as we have seen, the choice of (B2) leads naturally to the same RGE as the case of the finite system. The question is: Should there be some reason why the finite system picks out a particular renormalization scheme over all other choices?

Of the two schemes we easily denote the difference as whether or not a term such as

$$\frac{\partial}{\partial n}\Psi_1^2$$

is present in the RGE. This is equivalent to whether or not terms like

$$\int dV \psi_1^2 \text{ or } \int dV \psi_1 \psi_0$$

appear in the pertubative series for k_2^2. And the answer to this is, No.

From the procedure we have used to construct the perturbed eigenvalue, one may add to the definition of ψ_1 any constant multiple of ψ_0. So, we are able to make a transformation to a new solution:

$$\psi_1 \to \psi_1 + C\psi_0 \tag{B3}$$

and with a judicious choice of the constant C, we can make

$$\left\langle \epsilon^2 k_1^2 \int dV \psi_1 \psi_0 \right\rangle = 0. \tag{B4}$$

Thus all of the contribution to the perturbed eigenvalue can be made to come from only the surface integral in (A5).

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Hearing the shape of a general doubly connected domain in R^3 with impedance boundary conditions

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The basic problem in this paper is that of determining the geometry of a general doubly connected domain in R^3 together with an impedance condition on its inner bounding surface and another impedance condition on its outer bounding surface, from the complete knowledge of the eigenvalues $\{\lambda_j\}_{j=1}^{\infty}$ for the three-dimensional Laplacian using the asymptotic expansion of the spectral function $\theta(t) = \Sigma_{j=1}^{\infty} \exp(-t\lambda_j)$ for small positive t.

I. INTRODUCTION

The underlying problem is to deduce the precise shape of a membrane from the complete knowledge of the eigenvalues λ_j for the Laplace operator

$$\nabla^2 = \sum_{i=1}^{3} \left(\frac{\partial}{\partial x^i}\right)^2$$

in the $x^1x^2x^3$ space.

Let $\Omega \subseteq R^3$ be a simply connected bounded domain with a smooth bounding surface S. Consider the impedance problem

$$(\nabla^2 + \lambda)u = 0 \text{ in } \Omega, \quad \left(\frac{\partial}{\partial n} + \gamma\right)u = 0 \text{ on } S, \tag{1.1}$$

where $\partial/\partial n$ denotes differentiation along the inward pointing normal to S and γ is a positive constant. Denote its eigenvalues, counted according to multiplicity, by

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \lambda_3 \leqslant \cdots \leqslant \lambda_j \leqslant \cdots \to \infty \text{ as } j \to \infty. \tag{1.2}$$

The problem of determining the geometry of Ω and the impedance γ has been discussed recently in Refs. 1 and 2 from the asymptotic behavior of the spectral function

$$\theta(t) = \operatorname{tr}[\exp(-t\nabla^2)] = \sum_{j=1}^{\infty} \exp(-t\lambda_j) \quad \text{as } t \to 0. \tag{1.3}$$

Problem (1.1) has been investigated in Refs. 3, 1, 4, and 5 in the following special cases.

Case 1 [$\gamma = 0$ (Neumann problem)]:

$$\theta(t) = \frac{V}{(4\pi t)^{3/2}} + \frac{S}{16\pi t} + \frac{1}{12\pi^{3/2}t^{1/2}} \times \int_S H\,dS + a_0 + O(t^{1/2}) \quad \text{as } t \to 0. \tag{1.4}$$

Case 2 [$\gamma \to \infty$ (Dirichlet problem)]:

$$\theta(t) = \frac{V}{(4\pi t)^{3/2}} - \frac{S}{16\pi t} + \frac{1}{12\pi^{3/2}t^{1/2}} \times \int_S H\,dS + a_0 + O(t^{1/2}) \quad \text{as } t \to 0. \tag{1.5}$$

In these formulas, V and S are, respectively, the volume and the surface area of Ω while $H = \frac{1}{2}(1/R_1 + 1/R_2)$ is the mean curvature of S, where R_1, R_2 are the principal radii of curvature. Furthermore, it has been shown that the constant term a_0 in (1.4) and (1.5) has the following form:

$$a_0 = \begin{cases} \dfrac{7}{512\pi} \displaystyle\int_S \left(\frac{1}{R_1} - \frac{1}{R_2}\right)^2 dS, & \text{in the case of Neumann problem (see Ref. 1),} \\ \dfrac{1}{512\pi} \displaystyle\int_S \left(\frac{1}{R_1} - \frac{1}{R_2}\right)^2 dS, & \text{in the case of Dirichlet problem (see Ref. 5).} \end{cases}$$

In terms of the mean curvature H and Gaussian curvature $N = 1/R_1R_2$, then

$$a_0 = \begin{cases} \dfrac{7}{128\pi} \displaystyle\int_S (H^2 - N)ds, & \text{in the case of Neumann problem,} \\ \dfrac{1}{128\pi} \displaystyle\int_S (H^2 - N)ds, & \text{in the case of Dirichlet problem.} \end{cases} \tag{1.6}$$

The object of this paper is to discuss the following inverse problem: Let Ω be a general doubly connected domain in R^3 surrounding internally by a simply connected bounded domain Ω_1 with a smooth bounding surface S_1 and externally by a simply connected bounded domain Ω_2 with a smooth bounding surface S_2. Suppose that the eigenvalues (1.2) are given for the impedance problem

$$(\nabla^2 + \lambda)u = 0 \quad \text{in } \Omega, \tag{1.7}$$

$$\left(\frac{\partial}{\partial n_1} + \gamma_1\right)u = 0 \quad \text{on } S_1, \tag{1.8}$$

and

$$\left(\frac{\partial}{\partial n_2} + \gamma_2\right)u = 0 \quad \text{on } S_2, \tag{1.9}$$

where $\partial/\partial n_1$ and $\partial/\partial n_2$ denote differentiations along the inward pointing normals to S_1 and S_2, respectively, while γ_1 and γ_2 are positive constants. Determine the geometry of Ω as well as the impedances γ_1 and γ_2 from the asymptotic behavior of $\theta(t)$ for small positive t.

Note that problem (1.7)–(1.9) has been investigated recently by Zayed[6] in the special case where

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$$\Omega = \{(r,\theta,\phi): a \leqslant r \leqslant b,\ 0 \leqslant \theta \leqslant \pi,\ 0 \leqslant \phi \leqslant 2\pi\}$$

is a spherical shell.

II. STATEMENT OF RESULTS

Suppose that the outer bounding surface S_2 of the region Ω is given locally by infinitely differentiable functions $x^i = y^i(\sigma_2)$, $i = 1,2,3$, of the parameters σ_2^1, σ_2^2. If these parameters are chosen so that $\sigma_2^\alpha = \text{const}$, $\alpha = 1,2$ are lines of curvature, the first and second fundamental forms of S_2 can be written in the form:

$$\Pi_1(\sigma_2,\Delta\sigma_2) = g_{11}(\sigma_2)(\Delta\sigma_2^1)^2 + g_{22}(\sigma_2)(\Delta\sigma_2^2)^2$$

and

$$\Pi_2(\sigma_2,\Delta\sigma_2) = d_{11}(\sigma_2)(\Delta\sigma_2^1)^2 + d_{22}(\sigma_2)(\Delta\sigma_2^2)^2.$$

In terms of the coefficients $g_{11}, g_{22}, d_{11}, d_{22}$ the principal radii of curvature for S_2 and $R_{11} = g_{11}/d_{11}$ and $R_{22} = g_{22}/d_{22}$. Consequently, the mean curvature H_2 and Gaussian curvature N_2 of the outer bounding surface S_2 are

$$H_2 = \frac{1}{2}\left(\frac{1}{R_{11}} + \frac{1}{R_{22}}\right) \text{ and } N_2 = \frac{1}{R_{11}R_{22}}.$$

Similarly, suppose that the inner bounding surface S_1 of the region Ω is given locally by infinitely differentiable functions $x^i = y^i(\sigma_1)$, $i = 1,2,3$ of the parameters σ_1^1, σ_1^2. If these parameters are chosen so that $\sigma_1^\alpha = \text{const}$, $\alpha = 1,2$ are lines of curvature, the first and second fundamental forms of S_1 are

$$\Pi_1^*(\sigma_1,\Delta\sigma_1) = a_{11}(\sigma_1)(\Delta\sigma_1^1)^2 + a_{22}(\sigma_1)(\Delta\sigma_1^2)^2$$

and

$$\Pi_2^*(\sigma_1,\Delta\sigma_1) = b_{11}(\sigma_1)(\Delta\sigma_1^1)^2 + b_{22}(\sigma_1)(\Delta\sigma_1^2)^2.$$

In terms of the coefficients $a_{11}, a_{22}, b_{11}, b_{22}$ the principal radii of curvature are $r_{11} = a_{11}/b_{11}$ and $r_{22} = a_{22}/b_{22}$. Consequently, the mean curvature H_1 and Gaussian curvature N_1 of the inner bounding surface S_1 are

$$H_1 = \frac{1}{2}\left(\frac{1}{r_{11}} + \frac{1}{r_{22}}\right) \text{ and } N_1 = \frac{1}{r_{11}r_{22}}.$$

Let S_1 and S_2 be the surface areas of the inner and outer bounding surfaces S_1 and S_2, respectively, then the results of problem (1.7)–(1.8) can be summarized in the following cases.

Case 1 $(0 < \gamma_1 \ll 1,\ \gamma_2 \gg 1)$:

$$\theta(t) = \frac{V}{(4\pi t)^{3/2}} + \frac{1}{16\pi t}\left\{S_1 - \left(S_2 - 2\gamma_2^{-1}\int_{S_2} H_2\, dS_2\right)\right\} + \frac{1}{12\pi^{3/2}t^{1/2}}\left\{\int_{S_1}(H_1 - 3\gamma_1)dS_1 + \int_{S_2} H_2\, dS_2\right\}$$
$$+ \frac{1}{128\pi}\left\{7\int_{S_1}\left[(H_1 - 3\gamma_1)^2 - \left(N_1 - \frac{26}{7}\gamma_1 H_1 + \frac{47}{7}\gamma_1^2\right)\right]dS_1\right.$$
$$\left. + \int_{S_2}[H_2^2 - (N_2 - 16\gamma_2^{-1}H_2)]\,dS_2\right\} + O(t^{1/2}) \quad \text{as } t \to 0. \tag{2.1}$$

Case 2 $(\gamma_1 \gg 1,\ 0 < \gamma_2 \ll 1)$:

In this case the asymptotic expansion of $\theta(t)$ follows directly from (2.1) with the interchanges $S_1 \leftrightarrow S_2$, $\gamma_1 \leftrightarrow \gamma_2$.

Case 3 $(\gamma_1, \gamma_2 \gg 1)$:

$$\theta(t) = \frac{V}{(4\pi t)^{3/2}} - \frac{1}{16\pi t}\left\{\left(S_1 - 2\gamma_1^{-1}\int_{S_1} H_1\, dS_1\right) + \left(S_2 - 2\gamma_2^{-1}\int_{S_2} H_2\, dS_2\right)\right\}$$
$$+ \frac{1}{12\pi^{3/2}t^{1/2}}\left\{\int_{S_1} H_1\, dS_1 + \int_{S_2} H_2\, dS_2\right\} + \frac{1}{128\pi}\left\{\int_{S_1}[H_1^2 - (N_1 - 16\gamma_1^{-1}H_1)]\,dS_1\right.$$
$$\left. + \int_{S_2}[H_2^2 - (N_2 - 16\gamma_2^{-1}H_2)]\,dS_2\right\} + O(t^{1/2}) \quad \text{as } t \to 0. \tag{2.2}$$

Case 4 $(0 < \gamma_1, \gamma_2 \ll 1)$:

$$\theta(t) = \frac{V}{(4\pi t)^{3/2}} + \frac{S_1 + S_2}{16\pi t} + \frac{1}{12\pi^{3/2}t^{1/2}}\left\{\int_{S_1}(H_1 - 3\gamma_1)dS_1 + \int_{S_2}(H_2 - 3\gamma_2)dS_2\right\}$$
$$+ \frac{7}{128\pi}\left\{\int_{S_1}\left[(H_1 - 3\gamma_1)^2 - \left(N_1 - \frac{26}{7}\gamma_1 H_1 + \frac{47}{7}\gamma_1^2\right)\right]dS_1\right.$$
$$\left. + \int_{S_2}\left[(H_2 - 3\gamma_2)^2 - \left(N_2 - \frac{26}{7}\gamma_2 H_2 + \frac{47}{7}\gamma_2^2\right)\right]dS_2\right\} + O(t^{1/2}) \quad \text{as } t \to 0. \tag{2.3}$$

With reference to formulas (1.4)–(1.6) the asymptotic expansions (2.1)–(2.3) may be interpreted as follows.

(i) Ω is a general doubly connected domain in R^3 and we have the impedance boundary conditions (1.8), (1.9) with small/large impedances γ_1, γ_2 as indicated in the specifications of the four respective cases.

(ii) For the first four terms, Ω is a general doubly connected domain in R^3 of volume V.

In case 1, a part of its surface has area S_1, mean curvature $(H_1 - 3\gamma_1)$ and Gaussian curvature

$$\left(N_1 - \frac{26}{7}\gamma_1 H_1 + \frac{47}{7}\gamma_1^2\right)$$

together with Neumann boundary conditions, while the other part has area

$$\left(S_2 - 2\gamma_2^{-1}\int_{S_2} H_2\, dS_2\right),$$

mean curvature H_2 and Gaussian curvature $(N_2 - 16\gamma_2^{-1}H_2)$ together with Dirichlet boundary conditions.

In case 3, a part of its surface has area

$$\left(S_1 - 2\gamma_1^{-1}\int_{S_1} H_1\, dS_1\right),$$

mean curvature H_1 and Gaussian curvature $(N_1 - 16\gamma_1^{-1}H_1)$ together with Dirichlet boundary conditions, while the other part has area

$$\left(S_2 - 2\gamma_2^{-1}\int_{S_2} H_2\, dS_2\right),$$

mean curvature H_2 and Gaussian curvature $(N_2 - 16\gamma_2^{-1}H_2)$ together with Dirichlet boundary conditions.

In case 4, its surface has area $S_1 + S_2$. A part of this surface has mean curvature $(H_1 - 3\gamma_1)$ and Gaussian curvature

$$\left(N_1 - \frac{26}{7}\gamma_1 H_1 + \frac{47}{7}\gamma_1^2\right)$$

together with Neumann boundary conditions, while the other part has mean curvature $(H_2 - 3\gamma_2)$ and Gaussian curvature

$$\left(N_2 - \frac{26}{7}\gamma_2 H_2 + \frac{47}{7}\gamma_2^2\right)$$

together with Neumann boundary conditions.

III. FORMULATION OF THE MATHEMATICAL PROBLEM

In analogy with the two-dimensional membrane problem,[7] it is easy to show that $\theta(t)$ associated with problem (1.7)–(1.9) is given by

$$\theta(t) = \int\int_\Omega\int G(\mathbf{x},\mathbf{x};t)d\mathbf{x}, \tag{3.1}$$

where $G(\mathbf{x}_1,\mathbf{x}_2;t)$ is Green's function for the heat equation $\nabla^2 u = \partial u/\partial t$ subject to the impedance boundary conditions (1.8), (1.9) and the initial condition $G(\mathbf{x}_1,\mathbf{x}_2;t) \to \delta(\mathbf{x}_1 - \mathbf{x}_2)$ as $t\to 0$, where $\delta(\mathbf{x}_1 - \mathbf{x}_2)$ is the Dirac delta function located at the source point $\mathbf{x}_2$.

Let us write

$$G(\mathbf{x}_1,\mathbf{x}_2;t) = G_0(\mathbf{x}_1,\mathbf{x}_2;t) + \chi(\mathbf{x}_1,\mathbf{x}_2;t), \tag{3.2}$$

where

$$G_0(\mathbf{x}_1,\mathbf{x}_2;t) = (4\pi t)^{-3/2}\exp\{-|\mathbf{x}_1 - \mathbf{x}_2|^2/4t\}, \tag{3.3}$$

is the "fundamental solution" of the heat equation, while $\chi(\mathbf{x}_1,\mathbf{x}_2;t)$ is the "regular solution" chosen so that $G(\mathbf{x}_1,\mathbf{x}_2;t)$ satisfies the impedance boundary conditions (1.8) and (1.9).

On setting $\mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x}$ we find that

$$\theta(t) = V/(4\pi t)^{3/2} + K(t), \tag{3.4}$$

where V is the volume of Ω and

$$K(t) = \int\int_\Omega\int \chi(\mathbf{x},\mathbf{x};t)d\mathbf{x}. \tag{3.5}$$

In what follows, we shall use Laplace transforms with respect to "t," and use "s^2" as the Laplace transform parameter; thus we define

$$\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2) = \int_0^{+\infty} e^{-s^2 t}G(\mathbf{x}_1,\mathbf{x}_2;t)dt. \tag{3.6}$$

Consequently, we deduce that $\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ satisfies the membrane equation

$$(\nabla^2 - s^2)\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2) = -\delta(\mathbf{x}_1 - \mathbf{x}_2) \text{ in } \Omega, \tag{3.7}$$

together with the impedance conditions (1.8) and (1.9).

The asymptotic expansion of $K(t)$ as $t\to 0$ may then be deduced directly from the asymptotic expansion of $\overline{K}(s^2)$ as $s\to\infty$, where

$$\overline{K}(s^2) = \int\int_\Omega\int \bar{\chi}(\mathbf{x},\mathbf{x};s^2)d\mathbf{x}. \tag{3.8}$$

IV. CONSTRUCTION OF GREEN'S FUNCTION

It is well known[5] that the membrane equation (3.7) has the fundamental solution

$$\overline{G}_0(\mathbf{x}_1,\mathbf{x}_2;s^2) = \frac{\exp(-sr_{\mathbf{x}_1\mathbf{x}_2})}{4\pi r_{\mathbf{x}_1\mathbf{x}_2}} \text{ where } r_{\mathbf{x}_1\mathbf{x}_2} = |\mathbf{x}_1 - \mathbf{x}_2|$$

is the distance between the points $\mathbf{x}_1 = (x_1^1,x_1^2,x_1^3)$ and $\mathbf{x}_2 = (x_2^1,x_2^2,x_2^3)$ of the domain Ω. The existence of this solution enables us to construct integral equations for $\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ satisfying the impedance boundary conditions (1.8) and (1.9) for small/large impedances γ_1, γ_2. Therefore, Green's theorem gives the following cases.

Case 1 $(0<\gamma_1\ll 1, \gamma_2\gg 1)$:

$$\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2) = \frac{\exp(-sr_{\mathbf{x}_1\mathbf{x}_2})}{4\pi r_{\mathbf{x}_1\mathbf{x}_2}} + \frac{1}{2\pi}\int_{S_1}\overline{G}(\mathbf{x}_1,\mathbf{y};s^2)\left\{\frac{\partial}{\partial n_{1\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right] + \gamma_1\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right\}d\mathbf{y}$$
$$+ \frac{1}{2\pi}\int_{S_2}\frac{\partial}{\partial n_{2\mathbf{y}}}\overline{G}(\mathbf{x}_1,\mathbf{y};s^2)\left\{\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}} + \gamma_2^{-1}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right]\right\}d\mathbf{y}. \tag{4.1}$$

Case 2 $(\gamma_1\gg 1, 0<\gamma_2\ll 1)$:

In this case $\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ has the same form (4.1) with the interchanges $S_1\leftrightarrow S_2$, $\gamma_1\leftrightarrow\gamma_2$, and $\mathbf{n}_1\leftrightarrow\mathbf{n}_2$.

Case 3 $(\gamma_1,\gamma_2\gg 1)$:

In this case $\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ has the same form (4.1) except its second term which is different from the second term of (4.1). In case 3, the second term of $\overline{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ is equal to the negative of the third term of (4.1) with the interchanges $S_1\leftrightarrow S_2$, $\gamma_1\leftrightarrow\gamma_2$, and $\mathbf{n}_1\leftrightarrow\mathbf{n}_2$.

Case 4 ($0<\gamma_1, \gamma_2 \ll 1$):

In this case $\bar{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ has the same form (4.1) except its third term which is different from the third term of (4.1). In case 4, the third term of $\bar{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ is equal to the negative of the second term of (4.1) with the interchanges

$S_1 \leftrightarrow S_2$, $\gamma_1 \leftrightarrow \gamma_2$, and $\mathbf{n}_1 \leftrightarrow \mathbf{n}_2$.

On applying the iteration method (see Ref. 2) to the integral equation (4.1), we obtain the Green's function $\bar{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ which has the regular part:

$$\begin{aligned}\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2) = {} & \frac{1}{8\pi^2}\int_{S_1}\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}\left\{\frac{\partial}{\partial n_{1\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right]+\gamma_1\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right\}d\mathbf{y}+\frac{1}{8\pi^2}\int_{S_2}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}\right]\\ & \times\left\{\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}+\gamma_2^{-1}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{x}_2})}{r_{\mathbf{y}\mathbf{x}_2}}\right]\right\}d\mathbf{y}+\frac{1}{8\pi^2}\int_{S_1}\int_{S_1}\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}\cdot M_1(\mathbf{y},\mathbf{y}')\\ & \times\left\{\frac{\partial}{\partial n_{1\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right]+\gamma_1\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right\}d\mathbf{y}\,d\mathbf{y}'+\frac{1}{8\pi^2}\int_{S_2}\int_{S_2}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}\right]M_2(\mathbf{y},\mathbf{y}')\\ & \times\left\{\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}+\gamma_2^{-1}\frac{\partial}{\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right]\right\}d\mathbf{y}\,d\mathbf{y}'+\frac{1}{8\pi^2}\int_{S_1}\left\{\int_{S_2}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}\right]M_3(\mathbf{y},\mathbf{y}')d\mathbf{y}\right\}\\ & \times\left\{\frac{\partial}{\partial n_{1\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right]+\gamma_1\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right\}d\mathbf{y}'+\frac{1}{8\pi^2}\int_{S_2}\left\{\int_{S_1}\frac{\exp(-sr_{\mathbf{x}_1\mathbf{y}})}{r_{\mathbf{x}_1\mathbf{y}}}M_4(\mathbf{y},\mathbf{y}')d\mathbf{y}\right\}\\ & \times\left\{\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}+\gamma_2^{-1}\frac{\partial}{\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}'\mathbf{x}_2})}{r_{\mathbf{y}'\mathbf{x}_2}}\right]\right\}d\mathbf{y}', \end{aligned} \tag{4.2}$$

where

$$M_i(\mathbf{y},\mathbf{y}') = \sum_{\nu=0}^{\infty} K_i^{(\nu)}(\mathbf{y}',\mathbf{y}), \quad i=1-4, \tag{4.3}$$

$$K_1(\mathbf{y}',\mathbf{y}) = \frac{1}{2\pi}\left\{\frac{\partial}{\partial n_{1\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]+\gamma_1\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right\}, \tag{4.4}$$

$$K_2(\mathbf{y}',\mathbf{y}) = \frac{1}{2\pi}\left\{\frac{\partial}{\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]+\gamma_2^{-1}\frac{\partial^2}{\partial n_{2\mathbf{y}}\,\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]\right\}, \tag{4.5}$$

$$K_3(\mathbf{y}',\mathbf{y}) = \frac{1}{2\pi}\left\{\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}+\gamma_2^{-1}\frac{\partial}{\partial n_{2\mathbf{y}}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]\right\}, \tag{4.6}$$

and

$$K_4(\mathbf{y}',\mathbf{y}) = \frac{1}{2\pi}\left\{\frac{\partial^2}{\partial n_{1\mathbf{y}}\,\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]+\gamma_1\frac{\partial}{\partial n_{2\mathbf{y}'}}\left[\frac{\exp(-sr_{\mathbf{y}\mathbf{y}'})}{r_{\mathbf{y}\mathbf{y}'}}\right]\right\}. \tag{4.7}$$

Similarly, we can find $\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ for the other three cases.

On the basis of (4.2) the function $\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ will be estimated for large values of s together with small γ_1 and large γ_2. The case when $\mathbf{x}_1$ and $\mathbf{x}_2$ lie in the neighborhood of the inner bounding surface S_1 or in the neighborhood of the outer bounding surface S_2 is particularly interesting. To this end we shall use coordinates similar to those obtained in Sec. 3 of Ref. 2 as will be shown in the following section.

V. DIFFERENTIAL GEOMETRY OF THE BOUNDARY

Let n_1,n_2 be the minimum distances from a point $\mathbf{x}=(x^1,x^2,x^3)$ of the domain Ω to the bounding surfaces S_1,S_2, respectively. Letters $\mathbf{n}_1(\sigma_1)$, $\mathbf{n}_2(\sigma_2)$ denote the inward drawn unit normals to S_1,S_2, respectively. We note that the coordinates in the neighborhood of S_2 are in the same form as in Sec. 3 of Ref. 2 with the interchanges

$$\sigma^1 \leftrightarrow \sigma_2^1, \quad \sigma^2 \leftrightarrow \sigma_2^2, \quad n \leftrightarrow n_2, \quad h \leftrightarrow h_2,$$
$$I \leftrightarrow I_2, \quad C(I) \leftrightarrow C(I_2), \quad \delta^* \leftrightarrow \delta_2.$$

Thus we have the same formulas (3.1)–(3.4) of Sec. 3 in Ref. 2 with the interchanges $\mathbf{n}(\sigma) \leftrightarrow \mathbf{n}_2(\sigma_2)$, $n \leftrightarrow n_2$, $H \leftrightarrow H_2$, and $K \leftrightarrow N_2$. Similarly, the coordinates in the neighborhood of S_1 are similar to those obtained in Sec. 3 of Ref. 2 with the interchanges

$$\sigma^1 \leftrightarrow \sigma_1^1, \quad \sigma^2 \leftrightarrow \sigma_1^2, \quad n \leftrightarrow n_1, \quad h \leftrightarrow h_1,$$
$$I \to I_1, \quad C(I) \to C(I_1), \quad \delta^* \to \delta_1.$$

The only remark here is that the two unit normal vectors on S_1 and S_2 are in the opposite direction. Therefore, we have the same formulas (3.1)–(3.4) of Sec. 3 in Ref. 2 with the following interchanges:

$$\mathbf{n}(\sigma) \leftrightarrow \mathbf{n}_1(\sigma_1), \quad n \leftrightarrow n_1, \quad H \leftrightarrow H_1,$$
$$K \leftrightarrow N_1, \quad \Pi_1 \leftrightarrow \Pi_1^*, \quad \Pi_2 \leftrightarrow \Pi_2^*,$$

the plus sign of the second term of (3.1) by the minus sign, the minus sign of the second term of (3.2) by the plus sign, and the minus sign of the second term of (3.4) by the plus sign.

VI. SOME LOCAL EXPANSIONS

It now follows that the local expansions of the functions

$$\frac{\exp(-sr_{xy})}{r_{xy}}, \quad \frac{\partial}{\partial n_{1y}}\left[\frac{\exp(-sr_{xy})}{r_{xy}}\right], \quad \frac{\partial}{\partial n_{2y}}\left[\frac{\exp(-sr_{xy})}{r_{xy}}\right], \tag{6.1}$$

when the distance between x and y is small are very similar to those obtained in Secs. 4 and 5 of Ref. 2. Consequently, for small γ_1 and large γ_2 the local behavior of the following kernels

$$K_1(\mathbf{y}',\mathbf{y}), \quad K_4(\mathbf{y}',\mathbf{y}), \tag{6.2}$$

$$K_2(\mathbf{y}',\mathbf{y}), \quad K_3(\mathbf{y}',\mathbf{y}), \tag{6.3}$$

when the distance between y and y′ is small, follows directly from the knowledge of the local expansions of the functions (6.1). This follows from the definition of e^λ functions in small domains $C(I_1)$ and $C(I_2)$. Thus using methods similar to those obtained in Secs. 6–10 of Ref. 2, we can show that the functions (6.1) are e^λ functions with degrees $\lambda = -1, -2, -2$, respectively. Consequently, for small impedance γ_1 the functions (6.2) are e^λ functions with degrees $\lambda = 0, -1$ while for large impedance γ_2 the functions (6.3) are e^λ functions with degrees $\lambda = 0,1$.

Definition: If $\mathbf{x}_1,\mathbf{x}_2$ are points in a large domain $\Omega + S_1$ or $\Omega + S_2$, then we define

$$\hat{r}_{12} = \min_{\mathbf{y}} (r_{x_1,y} + r_{x_2,y}), \quad \text{if } \mathbf{y}\in S_1,$$

or

$$\hat{R}_{12} = \min_{\mathbf{y}} (r_{x_1,y} + r_{x_2,y}), \quad \text{if } \mathbf{y}\in S_2.$$

An $E^\lambda(\mathbf{x}_1,\mathbf{x}_2;s)$ function is defined and infinitely differentiable with respect to $\mathbf{x}_1$ and $\mathbf{x}_2$ when these points belong to a large domain $\Omega + S_1$ or $\Omega + S_2$ except when $\mathbf{x}_1 = \mathbf{x}_2 \in S_1$ or S_2. Thus the E^λ function has a similar local expansion of the e^λ function (see Ref. 2).

By the help of Secs. 8 and 9 in Ref. 2 it is easily seen that formula (4.2) is an $E^{-2}(\mathbf{x}_1,\mathbf{x}_2;s)$ function and consequently

$$\bar{G}(\mathbf{x}_1,\mathbf{x}_2;s^2) = O\{\hat{r}_{12}^{-2}\exp(-As\hat{r}_{12})\} + O\{\hat{R}_{12}^{-2}\exp(-Bs\hat{R}_{12})\}, \tag{6.4}$$

which is valid for $s\to\infty$ and for small γ_1 and large γ_2, where A and B are positive constants. Formula (6.4) shows that $\bar{G}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ is exponentially small for $s\to\infty$. Similar statements are true in the other three cases.

With reference to Sec. 10 in Ref. 2, if the e^λ expansions of the functions (6.1)–(6.3) are introduced into (4.2) and if we use formulas similar to (6.3) and (6.8) of Sec. 6 in Ref. 2, we obtain the following local behavior of $\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ when $\hat{r}_{12}$ or $\hat{R}_{12}$ is small which is valid for $s\to\infty$ and for small γ_1 and large γ_2:

$$\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2) = \bar{\chi}_1(\mathbf{x}_1,\mathbf{x}_2;s^2) + \bar{\chi}_2(\mathbf{x}_1,\mathbf{x}_2;s^2), \tag{6.5}$$

where, if $\mathbf{x}_1,\mathbf{x}_2$ belong to a sufficiently small domain $C(I_1)$, then

$$\bar{\chi}_1(\mathbf{x}_1,\mathbf{x}_2;s^2) = -\frac{1}{8\pi}\left[1-\gamma_1\left(\frac{\partial}{\partial\xi_1^3}\right)^{-1}\right]\frac{\exp(-s\hat{\rho}_{12})}{\hat{\rho}_{12}} + O\left\{\frac{\exp(-As\hat{\rho}_{12})}{\hat{\rho}_{12}}\right\}, \tag{6.6}$$

while, if $\mathbf{x}_1,\mathbf{x}_2$ belong to a sufficiently small domain $C(I_2)$, then

$$\bar{\chi}_2(\mathbf{x}_1,\mathbf{x}_2;s^2) = -\frac{1}{8\pi}\left[1-\gamma_2^{-1}\frac{\partial}{\partial\xi_1^3}\right]\frac{\exp(-s\hat{\rho}_{12})}{\hat{\rho}_{12}} + O\left\{\frac{\exp(-Bs\hat{\rho}_{12})}{\hat{\rho}_{12}}\right\}. \tag{6.7}$$

When $\hat{r}_{12}\geqslant\delta_1>0$ or $\hat{R}_{12}\geqslant\delta_2>0$ the function $\bar{\chi}(\mathbf{x}_1,\mathbf{x}_2;s^2)$ is of order $O(e^{-cs})$ as $s\to\infty$, $c>0$. Thus since $\lim \hat{r}_{12}/\hat{\rho}_{12} = 1$ or $\lim \hat{R}_{12}/\hat{\rho}_{12} = 1$ when $\hat{r}_{12}$ or $\hat{R}_{12}$ tends to zero, then we have the asymptotic formulas (6.6) and (6.7) with $\hat{\rho}_{12}$ in the small domains cases being replaced by $\hat{r}_{12}$ or $\hat{R}_{12}$ in the large domain $\Omega + S_1$ or $\Omega + S_2$, respectively. Similar formulas for the other three cases can be found.

VII. CONSTRUCTION OF OUR RESULTS

Since for $\xi^3\geqslant h_1>0$ or $\xi^3\geqslant h_2>0$ the function $\bar{\chi}_1(\mathbf{x},\mathbf{x};s^2)$ is of order $O(e^{-2Ash_1})$ while the function $\bar{\chi}_2(\mathbf{x},\mathbf{x};s^2)$ is of order $O(e^{-2Bsh_2})$, the integral over the region Ω of the function $\bar{\chi}(\mathbf{x},\mathbf{x};s^2)$ can be approximated in the following way [see (3.8)]:

$$\begin{aligned}\bar{K}(s^2) &= \int_{S_2}\int_{\xi^3=0}^{h_2}\bar{\chi}_2(\mathbf{x},\mathbf{x};s^2)[1-2\xi^3H_2+(\xi^3)^2N_2]d\xi^3dS_2 \\ &\quad - \int_{S_1}\int_{\xi^3=0}^{h_1}\bar{\chi}_1(\mathbf{x},\mathbf{x};s^2)[1-2\xi^3H_1 \\ &\quad + (\xi^3)^2N_1]d\xi^3\,dS_1 + O(e^{-2Ash_1}) \\ &\quad + O(e^{-2Bsh_2}) \quad \text{as } s\to\infty.\end{aligned} \tag{7.1}$$

If the e^λ expansions of $\bar{\chi}_1(\mathbf{x},\mathbf{x};s^2)$ and $\bar{\chi}_2(\mathbf{x},\mathbf{x};s^2)$ are introduced into (7.1) and by the help of formula (11.2) of Sec. 11 in Ref. 2 we deduce, after inverting Laplace transforms and using (3.4), that our results (2.1)–(2.3) have been constructed.

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Anomalies from geometric quantization of fermionic field theories

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Geometric quantization on (infinite-dimensional) graded symplectic manifolds is elaborated for a restricted class of phase spaces. The formalism includes the treatment of Fermionic field theories. The chiral anomaly [U(1)-anomaly] as well as the non-Abelian (covariant) anomaly of D-dimensional non-Abelian gauge theories is calculated in this framework.

I. INTRODUCTION

Using symplectic geometry on the classical phase space, geometric quantization[1] provides a coordinate-independent quantization scheme avoiding the ambiguity of operator ordering. In Ref. 2 it has been suggested to consider field theoretic anomalies in the context of this scheme. However, it is not clear in the literature,[3] to what extent geometric quantization is applicable to field theories. In Ref. 3 it was claimed (without proof) to yield the correct quantum field theory for linear systems and semiclassical approximations in general.

In previous work,[4] the authors have contributed to this discussion: Considering the nonconservation of the quantized chiral charge in time, they have shown how to calculate the chiral U(1) anomaly of a non-Abelian gauge theory in four dimensions within the geometric quantization scheme. As the chiral anomaly is a well-established feature of gauge theories, one can regard its determination to be a significant test for the application of geometric quantization to field theories.

In Ref. 3 the space $\mathscr{V}$ of solutions of the Dirac equation in a gauge background has been taken as the classical phase space for the Dirac system. In Ref. 4 a slightly different approach has been chosen: As in Ref. 3 the solutions $\Psi\in\mathscr{V}$ have been represented by their initial values $\Psi(x,t)|_{t=0}=:\psi_0(x)$. However, in accordance to the usual treatment of Fermionic field theories, the $\psi_\tau(x)$ have been regarded as *anticommuting* coordinates on a *graded* symplectic manifold.

Although graded manifolds are extensively used in the physics literature,[5,6] the subject of geometric quantization on such manifolds has been investigated systematically (to our knowledge) only in Ref. 7 and only up to the prequantum level. Hence, it suggests itself to deal with the formalism of geometric quantization on phase spaces with the structure of the one used in Ref. 4. This will be done in Sec. II of the present paper. More strictly speaking we will consider the quantization of a graded symplectic manifold $(X, \mathscr{A}, \omega)$ (in the notion of Ref. 7), where X is pointlike and $\mathscr{A}$ is the exterior algebra over the dual of a vector space. Results of Ref. 7 will be revisited as far as necessary to keep the paper self-contained. However, the consideration of a complex structure and the induced polarization as well as the construction of a quantum Hilbert space exceeds the material presented in Ref. 7.

In Sec. III of the present paper the geometric quantization formalism developed in Sec. II is applied to Dirac theory in even dimensions D. An appropriate polarization for a Dirac theory with gauge background is presented and the Fock space structure of the quantum Hilbert space is outlined.

A shortcoming of Ref. 4 was the restriction to the chiral anomaly in four space-time dimensions. In Sec. IV the chiral U(1) anomaly in arbitrary even D dimensions as well as the (covariant) non-Abelian anomaly are calculated. Generalizing Ref. 4 the results are in full agreement with the standard ones.[8] The calculation shows that the half-form contribution, corresponding to the transformation property of the measure in the Hilbert space, plays a crucial role in determining field theoretical anomalies. In the Appendix we will point out technical details of the calculations done in Sec. IV.

II. GRADED MANIFOLDS AND GEOMETRIC QUANTIZATION

Geometric quantization on the one hand and the theory of graded manifolds on the other hand are well established in the physics as well as in the mathematics literature. Already in 1975 Kostant showed in a remarkable work[7] that the notion of graded symplectic manifolds induces a natural connection between these two fields. However, with few exceptions (cf. Ref. 9) this connection has not received much attention in the literature. Hence, to the extent that we will need it later, we will start this section by repeating the main ideas of Ref. 7 in short. For more details on graded manifolds (supermanifolds) in finite and also in infinite dimensions we refer to Refs. 5 and 6.

Let A be an algebra decomposed into $A=A_0\oplus A_1$ such that $A_i\cdot A_j\subset A_{i+j}$, $i,j\in\mathbb{Z}_2$. We call $a_i\in A_i$ homogeneous element of A with degree $\mathrm{gr}(a_i)=i$; A is a graded (commutative) algebra over $\mathbb{Z}_2$, if the product of each two homogeneous elements a, $b\in A$ is graded commuting, i.e.,

$$a\cdot b=(-1)^{\mathrm{gr}(a)\mathrm{gr}(b)}b\cdot a. \tag{2.1}$$

In this sense A_0 and A_1 are referred to, respectively, as the even and the odd part of the algebra A.

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Let X be a smooth manifold and $\{U_i\}$ the set of all open subsets of X. Let A be a graded algebra, equipped with an appropriate topology and consider smooth functions $f_i: U_i \to A$. The set of these functions also forms a graded algebra under pointwise operations, denoted by $\mathscr{A}(U_i)$. For a pair $U_j \subset U_i$ the (natural) restriction

$$\rho_{U_j}^{U_i}: \mathscr{A}(U_i) \to \mathscr{A}(U_j), \qquad \rho_{U_j}^{U_i}(f_i) = f_i|_{U_j} \tag{2.2}$$

is an algebra homomorphism and the tupel $(X, \mathscr{A}(U_i), \rho_{U_j}^{U_i})$ is a special example of a sheaf. (For our purpose it is sufficient to consider a sheaf as an object of this type, for the exact definition we refer to Ref. 10.) If for an atlas $\{U_\alpha\}$ of X any function $f_\alpha \in \mathscr{A}(U_\alpha)$ can be written as

$$f_\alpha(x) = \tilde{f}_\alpha(x) + \sum_{n>0} \sum_{j_1 \cdots j_n} (\tilde{g}_\alpha(x))_{j_1 \cdots j_n} \theta_{j_1} \cdot \cdots \cdot \theta_{j_n}, \tag{2.3}$$

the sheaf $(X, \mathscr{A}(U_i), \rho_{U_j}^{U_i})$ together with this deomposition defines a graded manifold denoted by $(X, \mathscr{A})$. In (2.3) $x \in U_\alpha$ is a point, $\tilde{f}_\alpha$, $(\tilde{g}_\alpha)_{j_1 \cdots j_n}$, respectively, are usual $C^\infty(U_\alpha)$ functions and $\theta_{j_1} \cdot \cdots \cdot \theta_{j_n}$ are the generators of A. Note that $A = \mathbb{R}$ also fits into the definition of a graded algebra (with trivial odd part), hence each usual manifold X can also be considered as a graded manifold (X, C^∞). If in contrast $A = \mathrm{Gr}$ is a Grassmann algebra the corresponding $(X, \mathscr{G}_\infty)$ is also called a supermanifold.

For the application we have in mind let V be a vector space and V^* its dual. In the case of infinite dimensional V let the dual be defined with respect to some pairing (e.g., in the sense of Ref. 11). The exterior algebra $\oplus_n \Lambda^n(V^*)$ over this dual space is a $\mathbb{Z}_2$ graded algebra, with respect to the Λ product. If we consider $W := \oplus_n \Lambda^n(V^*)$ as a (trivial) sheaf over the pointlike manifold $X = \{p\}$, this defines a graded manifold

$$M_V := (\{p\}, W). \tag{2.4}$$

Here, the splitting (2.3) holds trivially, considering the elements of $V = \Lambda^1(V^*)$ as odd generators of W. As shown by Batchelor[6] the fact that V may be infinite dimensional does not spoil the construction. [In the same way as constructed above $\oplus_n \mathscr{S}^n(V^*)$, the symmetric tensor algebra of V^* defines a graded manifold $(\{p\}, \oplus_n \mathscr{S}^n(V^*))$ with trivial odd part. This example should be of interest in geometric quantization of Bosonic field theories, however it will be considered elsewhere.[12]]

For graded manifolds the notion of a tangent space is not so natural as for a usual manifold. Nevertheless it is possible to do differential geometry and proceed with geometric quantization by considering the space of all superderivations instead of $T(X)$. This space of superderivations $\mathrm{Der}(\mathscr{A}) \subset \mathrm{End}(\mathscr{A})$ over the algebra of functions $\mathscr{A}$ is defined as the space of all linear maps $\delta: \mathscr{A} \to \mathscr{A}$ obeying a graded Leibnitz rule:

$$\mathrm{Der}(\mathscr{A}) = \{\delta = \delta_0 + \delta_1 \in \mathrm{End}(\mathscr{A}) \mid \delta_k(f \cdot g) = \delta_k(f) \cdot g + (-1)^{\mathrm{gr}(f)\mathrm{gr}(\delta_k)} f \cdot \delta_k(g),\ k \in \mathbb{Z}_2\}, \tag{2.5}$$

where $\delta = \delta_0 + \delta_1$ is understood with respect to the naturally induced ($\mathbb{Z}_2$) grading of $\mathrm{End}(\mathscr{A})$. $\mathrm{Der}(\mathscr{A})$ does not define the tangent space of the graded manifold $(X, \mathscr{A})$, but generalizes the (algebraic) definition of $T(X)$ as the space of all derivations on $C^\infty(X)$. In coordinates (x_i, θ_j) on $(X, \mathscr{A})$ we have

$$\delta = \sum_i a_i \frac{\partial}{\partial x_i} + \sum_j b_j \frac{\partial}{\partial \theta_j} =: \sum_i a_i \partial_{x_i} + \sum_j b_j \partial_{\theta_j}, \tag{2.6}$$

with coefficients $a_i, b_j \in \mathscr{A}$. For $\delta, \tilde{\delta} \in \mathrm{Der}(\mathscr{A})$ the commutator between (homogeneous) superderivations naturally generalizes the commutator between vector fields

$$[\delta, \tilde{\delta}]_\pm := \delta\tilde{\delta} + (-1)^{\mathrm{gr}(\delta)\mathrm{gr}(\tilde{\delta})+1} \tilde{\delta}\delta. \tag{2.7}$$

In the example (2.4), superderivations δ of M_V are completely determined by their action on a base of V^* via linearity and Leibnitz rule. Thus $\mathrm{Der}(W)$ may be identified with $W \otimes V$ where the elements of V act on W as superderivations of homogeneous grading 1.

To generalize the definition of differential forms to graded manifolds (cf. Ref. 7) we consider (for all open $U_i \subset X$) the tensor algebra $T(U_i)$ of $\mathrm{Der}(\mathscr{A}(U_i))$ with coefficients in $\mathscr{A}(U_i)$ and denote by $T^m(U_i)$ the space of all m-tensors. Then the space of differential m-forms $\Omega^m(U_i, \mathscr{A}(U_i))$ is given as the set of all $\mathscr{A}(U_i)$-valued linear forms on $T^m(U_i)$ obeying a graded symmetry, specified below. Using the sheaf structure of $(X, \mathscr{A})$ we get globally $\Omega^m(X, \mathscr{A})$ as the space of all m-linear maps on $\mathrm{Der}(\mathscr{A})$ with values in $\mathscr{A}$, characterized by the additional graded symmetry condition on $\alpha \in \Omega^m(X, \mathscr{A})$

$$\alpha(\xi_1, \ldots, \xi_j, \xi_{j+1}, \ldots, \xi_m) = (-1)^{(\mathrm{gr}(\xi_j)+1)((\mathrm{gr}(\xi_{j+1})+1)} \alpha(\xi_1, \ldots, \xi_{j+1}, \xi_j, \ldots, \xi_m), \tag{2.8}$$

with $\xi_i \in \mathrm{Der}(\mathscr{A})$ homogeneous. (Note that our sign conventions coincide with Ref. 5 but not with Ref. 7.) For M_V all elements in V are of homogenous degree 1, so $\Omega^m(M_V)$ simplifies to the space of symmetric m-forms over V with values in W. Hence, denoting by $\mathscr{S}^m(V^*)$ the space of symmetric m-tensors over V^*

$$\Omega^m(M_V) = \mathscr{S}^m(V^*) \otimes W. \tag{2.9}$$

This may become more apparent in a coordinate description: Assume a basis set $\{e_i\}$ is given on V, so each $v \in V$ may be written as

$$v = \sum_i \theta_i(v) e_i. \tag{2.10}$$

The set of coordinates $\{\theta_i\}$ may be identified with the corresponding dual basis on V^*, i.e., $\theta_i(e_j) = \delta_{ij}$. Regarding θ_i as Grassmann numbers (anticommuting variables) elements of W become polynomials in θ_i. In these coordinates $\mathrm{Der}(W)$ is spanned by $\{\partial_{\theta_i}\}$ with

$$\partial_{\theta_i}(\theta_j)=\delta_{ij}. \tag{2.11}$$

Note that $\{\partial_{\theta_i}\}$ also determines a base of V that is anticommuting in contrast to $\{e_i\}$. For the construction of $\Omega^m(M_V)$ we denote the basis elements of $\mathscr{S}^1(V^*)$ by $d\theta_i$ with

$$d\theta_j(\partial_{\theta_i})=\partial_{\theta_i}\lrcorner\, d\theta_j=\delta_{ij}. \tag{2.12}$$

This notation becomes consistent if we take $d\theta_i$ to be commuting, in contrast to the θ_i. Then the symbol d coincides with the exterior derivative on W, in coordinates

$$d=d\theta_i\otimes\partial_{\theta_i}, \tag{2.13}$$

that acts as a derivative of grading 1 and is nilpotent ($d^2=0$). On a graded manifold we also have the notion of an interior derivative $\mathbf{i}_\xi$ with degree $\mathrm{gr}(\mathbf{i}_\xi)=\mathrm{gr}(\xi)+1$ defined as on a usual manifold by

$$\mathbf{i}_\xi\alpha(\xi_1,\ldots,\xi_{m-1})=\xi\lrcorner\,\alpha(\xi_1,\ldots,\xi_{m-1})=\alpha(\xi,\xi_1,\ldots,\xi_{m-1}). \tag{2.14}$$

Now let $A_{\mathbb{C}}=A\otimes\mathbb{C}$ be the complexification of the algebra A and let $\{U_\alpha\}$ be an open covering of X. Then a (complex) line bundle sheaf L over the graded maniold $(X,\mathscr{A})$ is locally determined as

$$L(U_\alpha)=\mathscr{A}_{\mathbb{C}}(U_\alpha)\otimes\tau_\alpha. \tag{2.15}$$

Here, τ_α are even generators of $A_{\mathbb{C}}$ with invertible transition functions $c^{\alpha\beta}\in\mathscr{A}(U_\alpha\cap U_\beta)$ given by $\tau_\alpha=c^{\alpha\beta}\tau_\beta$. Using the sheaf structure of $(X,\mathscr{A})$ this can be globalized. The space of sections of a line bundle L over a graded manifold is defined as in the usual case and will be denoted by $\Gamma(L)\equiv L(X)$. For geometric quantization L has to carry a Hermitian sturcture, i.e., a bilinear, Hermitian operation

$$(\cdot,\cdot)L\times L\to\mathscr{A}_{\mathbb{C}}, \tag{2.16}$$

mapping pairs of sections $\mathscr{S}(x)$, $\mathscr{T}(x)\in\Gamma(L)$ smoothly to a section $(\mathscr{S},\mathscr{T})(x)$ of the trivial line bundle $\mathscr{A}_{\mathbb{C}}$ over $(X,\mathscr{A})$. As for usual manifolds a connection ∇ on a line bundle sheaf L can be written as a map $\nabla_\xi: L\to L$, locally given by

$$\nabla_\xi\mathscr{S}=\xi\mathscr{S}+(\mathbf{i}_\xi\vartheta)\mathscr{S}\quad\text{for any }\xi\in\mathrm{Der}(\mathscr{A}), \tag{2.17}$$

where $\vartheta\in\Omega^1(\mathscr{A})$ has degree $\mathrm{gr}(\vartheta)=1$. The curvature of the connection then is $\mathrm{curv}\nabla=d\vartheta$ [with d given by (2.13)] and a Hermitian structure on a line bundle sheaf is said to be compatible with the connection, if

$$\xi(\mathscr{S},\mathscr{T})=(\nabla_\xi\mathscr{S},\mathscr{T})+(\mathscr{S},\nabla_\xi\mathscr{T}). \tag{2.18}$$

For more details we refer to Ref. 7.

Symplectic mechanics on a graded manifold proceeds as for usual manifolds: $\omega\in\Omega^2(X,\mathscr{A})$ is called a graded symplectic form, if it is even with respect to the grading of $\mathscr{A}$, closed ($d\omega=0$) and (weakly) nondegnerated on $\mathrm{Der}(\mathscr{A})$ [i.e., if $\omega(V,W)=0$ for all $V\in\mathrm{Der}(\mathscr{A})$ then $W=0$, cf. Ref. 11]. Then due to the graded Darboux theorem there exist local coordinates with

$$\omega=\frac{1}{2}\sum_{ij}f^{ij}dx_i\,dx_j+\frac{1}{2}\sum_{ij}g^{ij}d\theta_i\,d\theta_j, \tag{2.19}$$

where the matrices f^{ij} (antisymmetric) and g^{ij} (symmetric) are constant and of grading 0. Also there is a graded Poincaré lemma that (locally) guarantees the existence of Θ with $\omega=d\Theta$. For M_V the Darboux theorem and the Poincaré lemma hold globally and the f^{ij} in (2.19) vanish. To generalize the Poisson algebra from $C^\infty(X)$ to $\mathscr{A}$ one assigns via

$$\xi_F\lrcorner\,\omega+dF=0, \tag{2.20}$$

a Hamiltonian vector field $\xi_F\in\mathrm{Der}(\mathscr{A})$ to each obserable $F\in\mathscr{A}$. Then the Poisson algebra over $\mathscr{A}$ is given by

$$\{F,G\}=(-1)^{\mathrm{gr}(F)}\xi_F G=(-1)^{\mathrm{gr}(F)1}\xi_F\lrcorner\,\xi_G\lrcorner\,\omega, \tag{2.21}$$

with $\xi_F G=\xi_F\lrcorner\,dG$. In Darboux coordinates this is

$$\{F,G\}=\sum_{ij}(f^{ij})^{-1}\frac{\partial F}{\partial x_i}\frac{\partial G}{\partial x_j}+(-1)^{\mathrm{gr}(F)}\sum_{ij}(g^{ij})^{-1}\frac{\partial F}{\partial\theta_i}\frac{\partial G}{\partial\theta_j}. \tag{2.22}$$

This includes the usual Poisson bracket and also gives an anticommutator on the level of classical mechanics.

The first aim of geometric quantization is to associate to each observable $F\in\mathscr{A}$ an operator $\mathscr{O}_F$, acting on sections of a complex line bundle sheaf L over the graded symplectic manifold $(X,\mathscr{A},\omega)$ such that a representation of the Poisson algebra is provided and the unit element $1\in\mathscr{A}$ is represented as the unit operator:

$$[\mathscr{O}_F,\mathscr{O}_G]_\pm=-i\hbar\mathscr{O}_{\{F,G\}},\qquad \mathscr{O}_1=\mathbf{1}. \tag{2.23}$$

Such a representation is called prequantization. If we consider a usual symplectic manifold with $[\omega]$ integral, Weil's theorem guarantees that there exists a Hermitian line bundle L over X with a connection ∇ such that ∇ is compatible with the Hermitian structure on L and induces the symplectic form by $\omega=\mathrm{curv}\,(\nabla)$. For a graded manifold $(X,\mathscr{A})$ such a Hermitian line bundle sheaf has been shown in Ref. 7 (cf. Sec. 6.3) to exist if X has trivial cohomology. This is the case for our application (2.4); moreover, the line bundle over M_V can be chosen trivial, i.e., $L_V=W\otimes\mathbb{C}$. The prequantum operator on such a line bundle sheaf is then given by

$$\mathscr{O}_F:\Gamma(L)\to\Gamma(L),\qquad \mathscr{O}_F=-i\hbar\nabla_{\xi_F}+F, \tag{2.24}$$

where the covariant derivative ∇_ξ may be written as

$$\nabla_\xi=\xi-(i/\hbar)\xi\lrcorner\,\Theta. \tag{2.25}$$

However, full quantization demands an irreducible representation of the Heisenberg subalgebra (cf. Ref. 1), not given by (2.24). On a usual manifold X this problem is solved by choosing a polarization (Lagrangian subspace) $P\subset T^{\mathbb{C}}(X)$ of the complexified tangent space. An appropriate polarization for geometric quantization is provided

by a Kähler structure[13] on X. We use the notion of Ref. 3 and define an (almost) Kähler structure on X as a linear involution $J:T(X)\to T(X)$ with

$$J^2=-1,\quad \omega(J(\xi),J(\eta))=\omega(\xi,\eta). \tag{2.26}$$

If one can choose on X local coordinates $\{z_k,z_k^+\}$ solving over $T^{\mathbb{C}}(X)$ the eigenvalue problem

$$J\left[\frac{\partial}{\partial z_k}\right]=+i\left(\frac{\partial}{\partial z_k}\right),\quad J\left[\frac{\partial}{\partial z_k^+}\right]=-i\left(\frac{\partial}{\partial z_k^+}\right). \tag{2.27}$$

This defines a Kähler polarization P spanned by the eigenvectors $\partial/\partial z_k^+ =:\partial_{z_k^+}$. This description of a Kähler structure easily generalizes to graded manifolds given by an automorphism $J:\mathrm{Der}(\mathscr{A})\to\mathrm{Der}(\mathscr{A})$ obeying (2.26). A Kähler polarization on a graded manifold is then determined by

$$P=\mathrm{Span}(\{\partial_{z_k^+}\})\subset\mathrm{Der}(\mathscr{A})\ \text{with}\ J[\partial_{z_k^+}]=-i(\partial_{z_k^+}). \tag{2.28}$$

To fulfill the irreducibility condition we have to represent classical observables as operators on the space of polarized sections

$$\Gamma^P(L)=\{\mathscr{S}\in\Gamma(L)\,|\,\nabla_\xi\mathscr{S}=0\ \text{for all}\ \xi\in P\}. \tag{2.29}$$

For a Kähler polarization this means that the wave functions $\mathscr{S}\in\Gamma^P(L)$ have to be holomorphic sections, i.e., covariantly constant under $\nabla_{z_k^+}$.

On a usual ($2m$-dimensional) manifold X the symplectic form ω induces a natural volume element $(\omega)^m$. Using this for integration over X the Hermitian structure (2.16) on L extends to an inner product on $\Gamma(L)$ by

$$\langle\cdot,\cdot\rangle:\Gamma(L)\times\Gamma(L)\to\mathbb{C},\qquad \langle\xi,\eta\rangle=\int(\xi,\eta)(\omega)^m. \tag{2.30}$$

Such is not the case on a graded manifold, where integration over forms is not defined directly. Due to Berezin[5] integration over anticommuting variables is identified with differentiation. A naive identification would yield a coordinate dependent integral. However, considering the symplectic graded manifold M_V and a complex structure J defined on it Berezin's idea can be used to determine a coordinate independent integration: On M_V the symplectic form ω determines a map τ between superderivations and one-forms by

$$\tau:\mathrm{Der}(M_V)\to\Omega^1(M_V),\qquad \tau(\xi):=\xi\lrcorner\omega. \tag{2.31}$$

On the other hand the symplectic form and the complex structure yield an antisymmetric tensor field g on $\mathrm{Der}\,(M_V)$ by

$$g(\xi,\eta)=\omega(J(\xi),\eta),\ \xi,\eta\in\mathrm{Der}(M_V). \tag{2.32}$$

We note that $\omega\in\Omega^2(M_V)$ and hence $g\in W\otimes\Lambda^2(V^*)$, so we can define an antisymmetric form $\omega'\in W\otimes\Lambda^2(V)$

$$\omega'(\alpha,\beta)=g(\tau^{-1}\alpha,\tau^{-1}\beta),\ \alpha,\beta\in\Omega^1(M_V). \tag{2.33}$$

For $2m$-dimensional V, the m-fold tensor product $(\omega')^m\in W\otimes\Lambda^{2m}(V)$ provides a natural volume element for the integration of functions over M_V, i.e., integration of sections $F\in\Gamma(L_V)$ in the following way. We have

$$F\cdot(\omega')^m\in W\otimes\Lambda^{2m}(V) \tag{2.34}$$

and the integration is carried out applying the $\Lambda^{2m}(V)$ part as product of superderivations to W. This yields a coordinate independent map

$$\int\cdot(\omega')^m:\Gamma(L_V)\to\mathbb{C}, \tag{2.35}$$

that gives in coordinates the Berezin integral with $\sqrt{\det g_{ij}}$ used as integration measure. We note that this generalizes to infinite dimensions (cf. Chap. I.3 of Ref. 14).

In contrast to $\Gamma(L)$ on the space of polarized sections $\Gamma^P(L)$ the natural volume element $(\omega)^m$ [respectively, $(\omega')^m$] does, in general, not induce a pairing by integration. Therefore, it is necessary to introduce the notion of half-forms.[1] Essentially a half-form on a usual manifold X is a function on the bundle of frames $\mathscr{F}^P(X)$ spanning the polarization P:

$$\nu:\mathscr{F}^P(X)\to\mathbb{C}, \tag{2.36}$$

which transforms under right group actions g on P according to

$$\nu\circ g=(\det_P g)^{-1/2}\nu. \tag{2.37}$$

Roughly speaking ν reflects the transformation property of the measure in the Hilbert space build from the space of polarized sections $\Gamma^P(L)$. For infinite-dimensional manifolds one furthermore has to choose a proper regularization to make the determinant well defined. The notion of half-forms can also be applied to our graded manifold $M_V(\{p\},W)$:

$$\nu:\mathscr{F}^P(W)\to W, \tag{2.38}$$

where $\mathscr{F}^P$ is the frame bundle of the polarization $P\subset\mathrm{Der}(W)$ and ν transforms under group actions according to (2.37).

Quantum states are now taken as products of a (normalized) polarized section $\mathscr{S}\in\Gamma^P(L)$ and a half-form ν corresponding to the polarization P. The quantum operator $\hat{F}$ of a classical observable $F\in\mathscr{A}$ then becomes the sum of the prequantum action $\mathscr{O}_F$ on $\mathscr{S}$ and the Lie derivative of ν with respect to the Hamiltonian vector field ξ_F:

$$\hat{F}(\mathscr{S}\nu)=\mathscr{O}_F\mathscr{S}\cdot\nu+i\mathscr{S}\cdot\mathscr{L}_{\xi_F}\nu. \tag{2.39}$$

Note that this gives the right quantum operator only if F respects the polarization in the sense that

$$[\xi_F,P]\subset P. \tag{2.40}$$

In the case of a Kähler polarization, a holomorphic projection[15] is needed to obtain the correct quantum operator

for observables not respecting the polarization. However, this will not be crucial for our following considerations.

III. GEOMETRIC QUANTIZATION OF DIRAC THEORY

To elaborate geometric quantization for a Dirac field we consider (according to Ref. 3) the space of solutions of the (massless) Dirac equation

$$\gamma^{\mu}(i\partial_{\mu}+A_{\mu}(x,t))\Psi(x,t)=0, \tag{3.1}$$

in D space-time dimensions in a non-Abelian background. The elements Ψ of this space are complex D-spinors and the field $A(x,t)$ is regarded as an external gauge connection $A(x,t)=A_a(x,t)T^a$ with T^a generating the gauge group. Our conventions are similar as in Ref. 4 and can be found in the Appendix, Eq. (A1). A solution of (3.1) is uniquely determined by its value $\psi_\tau(x)$ at a fixed time τ via

$$\Psi(x,t)\,|_{t=\tau}=:\psi_\tau(x), \tag{3.2}$$

what respects the linear structure of the solution space. An inner product between solutions of (3.1) is given by

$$\Psi\odot\tilde{\Psi}:=\int_{\Sigma_\tau}\psi_\tau^+(x)\,\tilde{\psi}_\tau(x)d^{D-1}x, \tag{3.3}$$

where Σ_τ denotes the $t=\tau$ hypersurface. This fixes the space under consideration:

$$\mathscr{V}:=\{\Psi \text{ solution of (3.1)}\,|\,\Psi\odot\Psi<\infty\}. \tag{3.4}$$

As explained above (2.4), this yields a graded manifold with the dual $\mathscr{V}^*$ determined by (3.3):

$$M_{\mathscr{V}}=(\{p\},\oplus_n\Lambda^n(\mathscr{V}^*)). \tag{3.5}$$

The $(D-1)$ dimensional δ-functions span (formally) $\mathscr{V}^*$ assigning to each $\Psi\in\mathscr{V}$ its value $\psi_\tau(x)$ at some space point x. As explained in (2.10) and (2.11) we use $\psi_\tau(x)$ as anticommuting coordinates on $M_{\mathscr{V}}$. [Note that our notation does not distinguish between $\psi_\tau(x)$ as elements of $\mathscr{V}^*$ and as functions on Σ_τ!] With the symplectic form

$$\omega=i\int_{\Sigma_\tau}d\psi_\tau^+(x)d\psi_\tau(x)d^{D-1}x \tag{3.6}$$

on $M_{\mathscr{V}}$ the Poisson bracket, (2.22) yields the well-known equal time anticommutator:

$$\{\psi_\tau(x),\psi_\tau^+(x')\}_+=-\xi_{\psi_\tau(x)}\psi_\tau^+(x')=+i\delta(x-x'). \tag{3.7}$$

Here, $\mathscr{V}$ is per construction a complex vector space, but the Kähler polarization with respect to the natural complex structure is not acceptable from the physical point of view: It would lead to an energy spectrum that is unbounded from below. For the free theory ($A=0$) an appropriate polarization is given in Ref. 1. There the operator

$$B_{\mathrm{fr}}=\gamma^0\gamma^j i\partial_j \tag{3.8}$$

is used to split the space of solutions of the free Dirac equation $\mathscr{V}$ into a positive and a negative frequency part in order to define a complex structure by

$$J_{\mathrm{fr}}[\psi_\lambda]=i\,\mathrm{sign}(\lambda)\psi_\lambda \text{ for eigenstates } B_{\mathrm{fr}}\psi_\lambda(x)=\lambda\psi_\lambda(x). \tag{3.9}$$

A natural generalization of (3.8) for a theory in a background field is

$$B_t=\gamma^0\gamma^j(i\partial_j+A_j(x,t)). \tag{3.10}$$

We proceed in analogy to the free case and decompose at $t=\tau$ the function ψ_τ into a formal sum of eignfunctions φ_n^τ of the Hermitian operator B_τ

$$\psi_\tau=\sum_n c_n^\tau\varphi_n^\tau \quad \text{with } B_\tau\varphi_n^\tau(x)=\lambda_n^\tau\varphi_n^\tau(x). \tag{3.11}$$

In contrast to the free case, λ_n^τ determines the time evolution of φ_n^τ only up to first order, nevertheless $\{\varphi_n^\tau\}$ provides a basis of $\mathscr{V}$. Considering (3.11) one should note that the deomposition is not discrete, so the sum over φ_n is only formal and has to be understood as an integration.

In the corresponding coordinate system $\{c_n^\tau\}$ we now can define the complex structure J^τ by

$$\begin{aligned}J^\tau\left[\frac{\partial}{\partial c_n^\tau}\right]&=+i\,\mathrm{sign}(\lambda_n^\tau)\frac{\partial}{\partial c_n^\tau},\\ J^\tau\left[\frac{\partial}{\partial c_n^{\tau+}}\right]&=-i\,\mathrm{sign}(\lambda_n^\tau)\frac{\partial}{\partial(c_n^\tau)^+}.\end{aligned} \tag{3.12}$$

This complex structure explicitly depends on τ. As τ can be chosen arbitrarily it defines a time-dependent complex structure $J(t)$ by $J(t)\,|_{t=\tau}:=J^\tau$. To describe this in a small neighborhood of τ, i.e., for $t=\tau+\delta t$, we use the (unitary) transformation matrix $\beta_{mn}^{(\tau,t)}$ between the eigenstates of B_τ and B_t:

$$\varphi_n^t=\sum_m\beta_{mn}^{(\tau,t)}\varphi_m^\tau. \tag{3.13}$$

Then we have in $\{c_n^\tau\}$ coordinates the complex structure

$$J(\tau+\delta t)\left[\frac{\partial}{\partial c_n^\tau}\right]=i\sum_{lm}\beta_{nl}^{(\tau,t)}\mathrm{sign}(\lambda_l^t)(\beta_{lm}^{(\tau,t)})^{-1}\frac{\partial}{\partial c_m^\tau}+\sigma(\delta t^2), \tag{3.14}$$

with a similar expression for $c_n^{\tau+}$. The complex structure is also a functional of the gauge background $[J(t)=J(t)[A]]$ and transforms covariantly with respect to local (fixed time) gauge transformations $\alpha(x)=\alpha_a(x)T^a$:

$$e^{i\alpha(x)}J(t)[A]e^{-i\alpha(x)}=J(t)[\rho_\alpha A]. \tag{3.15}$$

The Kähler polarization P^τ, determined by $J(t)\,|_{t=\tau}$ is then given as

$$P^\tau=\mathrm{span}\left(\left\{\frac{\partial}{\partial c_n^\tau}\middle|\lambda_n^\tau<0\right\}\oplus\left\{\frac{\partial}{\partial c_n^{\tau+}}\middle|\lambda_n^\tau>0\right\}\right) \tag{3.16}$$

and naturally induces holomorphic (anticommuting) coordinates

$$z_n^\tau=\begin{cases}c_n^\tau, & \lambda_n^\tau>0,\\ c_n^{\tau+}, & \lambda_n^\tau<0,\end{cases}\qquad (z_n^\tau)^+=\begin{cases}c_n^\tau, & \lambda_n^\tau<0,\\ c_n^{\tau+}, & \lambda_n^\tau>0.\end{cases} \tag{3.17}$$

In order to simplify our notation we will suppress the index τ in the sequel whenever this is possible.

We proceed in the coordinates $\{z_n, z_n^+\}$ on the graded manifold $M_{\mathscr{V}}$ where the symplectic form (3.6) is

$$\omega = i \sum_n dz_n^+ dz_n, \tag{3.18}$$

and Θ can be chosen as

$$\Theta = \frac{i}{2}\left(\sum_n z_n^+ dz_n + \sum_n dz_n^+ z_n \right). \tag{3.19}$$

According to (2.29) polarized sections $\mathscr{S} \in \Gamma^P(L_{\mathscr{V}})$ have to obey

$$\nabla_{\partial_{z_k^+}} \mathscr{S}(z, z^+) = 0. \tag{3.20}$$

Hence with (2.25) and Θ given in (3.19) (see also Ref. 1) we obtain

$$\mathscr{S}(z, z^+) = \sigma(z) \exp\left(-\frac{1}{2} \sum_n z_n z_n^+ \right), \tag{3.21}$$

where the $\sigma(z)$ are holomorphic functions. On the (trivial) line bundle $L_{\mathscr{V}}$ over $M_{\mathscr{V}}$ the Hermitian structure defined by

$$(\mathscr{S}, \mathscr{T}) = \mathscr{S}^+ \cdot \mathscr{T}, \qquad \mathscr{S}, \mathscr{T} \in \Gamma(L_{\mathscr{V}}) \tag{3.22}$$

is compatible with the covariant derivative (2.25) on $L_{\mathscr{V}}$ (cf. Ref. 1, respectively, Ref. 7). It extends (formally) to the inner product on the space Γ of sections of $L_{\mathscr{V}}$:

$$\langle \mathscr{S}(z, z^+), \mathscr{T}(z, z^+) \rangle = \lim_{m \to \infty} \int (\omega')^m (\mathscr{S}, \mathscr{T})(z, z^+). \tag{3.23}$$

To make this formal definition meaningful we can approximate $\mathscr{V}$ as a sequence of finite-dimensional vector spaces V_n as proposed in Refs. 14 and 3. However, as a pairing between sections $\mathscr{S} \in \Gamma^P(L)$ (3.23) is well defined if it is understood in terms of the Fock space structure given below.

Geometric quantization of the Dirac equation means to determine the quantum operators (2.39) of any observable and apply it to polarized sections $\mathscr{S} \in \Gamma^P(L_{\mathscr{V}})$. For the coordinate functions z_k, z_k^+ as classical observables the half-form contribution $\mathscr{L}_{\xi_F} \nu$ in (2.39) vanishes for an appropriate normalization of the half-form ν [cf. (3.33)] and we obtain

$$\begin{aligned} \hat{z}_k^+ \mathscr{S}(z, z^+) \nu &= (\partial_{z_k} \sigma(z)) \exp\left(-\frac{1}{2} \sum_n z_n z_n^+ \right) \nu, \\ \hat{z}_k \mathscr{S}(z, z^+) \nu &= (z_k \cdot \sigma(z)) \exp\left(-\frac{1}{2} \sum_n z_n z_n^+ \right) \nu. \end{aligned} \tag{3.24}$$

This coincides with the well-known holomorphic representation of Fermionic field theory (cf. Refs. 16 and 14). We define the vacuum state $|0\rangle \in \Gamma^P(L_{\mathscr{V}})$ by

$$|0\rangle = \left(\prod_n z_n \right) \exp\left(-\frac{1}{2} \sum_m z_m z_m^+ \right) \nu = \left(\prod_n z_n \right) \nu, \tag{3.25}$$

where $\prod z_n$ means the formal product over all coordinates z_n. This yields formally

$$\langle 0 | 0 \rangle = 1, \tag{3.26}$$

what may be regarded either as a definition or as the result of a limiting procedure defining (3.23) and (3.25) properly. Then (3.24) gives the interpretation of $\hat{z}_k^+$ and $\hat{z}_k$, respectively, as creation and annhilation operators

$$\begin{aligned} \hat{z}_k |0\rangle &= 0, \\ \hat{z}_k^+ |0\rangle &=: |k\rangle, \end{aligned} \tag{3.27}$$

for they fulfill the (usual) anticommutation relations

$$\begin{aligned} [\hat{z}_k, \hat{z}_l]_+ &= [\hat{z}_k^+, \hat{z}_l^+]_+ = 0, \\ [\hat{z}_k^+, \hat{z}_l]_+ &= \delta_{kl}. \end{aligned} \tag{3.28}$$

Together with (3.26) this yields the orthonormality relation

$$\langle k | l \rangle = \delta_{kl}. \tag{3.29}$$

The construction of the Fock space given above corresponds to the polarization P^t only at $t = \tau$. To extend this to a time $t = \tau + \delta t$ we use (3.14) to define holomorphic coordinates by

$$\begin{aligned} z_n^t &= \begin{cases} c_m^\tau \beta_{mn}^{(\tau,t)}, & \lambda_n^t > 0, \\ (\beta_{nm}^{(\tau,t)})^{-1} c_m^{\tau +}, & \lambda_n^t < 0, \end{cases} \\ (z_n^t)^+ &= \begin{cases} c_m^\tau \beta_{mn}^{(\tau,t)}, & \lambda_n^t < 0, \\ (\beta_{nm}^{(\tau,t)})^{-1} c_m^{\tau +}, & \lambda_n^t > 0, \end{cases} \end{aligned} \tag{3.30}$$

what in some sense corresponds to the interaction picture of quantum mechanics. The dynamics of the system then is determined by the (time-dependent) Hamiltonian

$$\begin{aligned} H_t &= \int_{\Sigma_t} \Psi^+(x,t) \gamma^0 \gamma^j (i\partial_j + A_j(x,t)) \Psi(x,t) d^3x \\ &= \sum_n |\lambda_n^t| (z_n^t)^+ z_n^t, \end{aligned} \tag{3.31}$$

where we choose the $A_0 = 0$ gauge for sake of simplicity. At $t = \tau$ the corresponding Hamiltonian vector field of H_t is given by

$$\xi_{H_\tau} = +i \sum_n |\lambda_n^\tau| \left((z_n^\tau)^+ \frac{\partial}{\partial (z_n^\tau)^+} - z_n^\tau \frac{\partial}{\partial z_n^\tau} \right), \tag{3.32}$$

preserving the Kähler polarization J^τ. To quantize H_τ we have to consider further the half-form contributions. Choosing a reference half-form ν_0 on P^τ (3.16) normed by $\nu_0(\partial_{z_1^+}, \ldots, \partial_{z_k^+}, \ldots) = 1$ quantum states are determined as

$$|\Sigma\rangle = \mathscr{S}(z, z^+) \nu_0 = \exp\left(-\frac{1}{2} \sum z_n^+ z_n \right) \sigma(z) \nu_0. \tag{3.33}$$

Then we obtain for the quantum operator $\hat{H}_\tau$

$$\hat{H}_\tau|\Sigma\rangle = -e^{-1/2\Sigma z_n^+ z_n}\left(\sum_k |\lambda_k^\tau| z_k^\tau \frac{\partial}{\partial z_k^\tau}\sigma(z^\tau)\right)\nu_0$$
$$-\tfrac{1}{2}[\mathrm{Tr}_{P^\tau}(\mathscr{L}_{\xi_{H_\tau}})]\cdot\nu_0$$
$$= +e^{-1/2\Sigma z_n^+ z_n}\left(\sum_k |\lambda_k^\tau|\frac{\partial}{\partial z_k^\tau} z_k^\tau\sigma(z^\tau)\right)\nu_0$$
$$-\frac{1}{2}\sum_n |\lambda_n^\tau|\,|\Sigma\rangle. \tag{3.34}$$

This confirms the interpretation (3.27) of $\hat{z}_k^+ \hat{=} \partial/\partial z_k$ as creation operator of a one-particle state in Fock space with energy $\lambda_n > 0$. The vacuum contribution

$$\langle 0|\hat{H}_\tau|0\rangle_\tau = -\frac{1}{2}\sum_n |\lambda_n^\tau| \tag{3.35}$$

of the Hamiltonian may be compensated by a redefinition of the classical Hamiltonian due to

$$H_\tau \to H_\tau + \frac{1}{2}\sum_n |\lambda_n^\tau|,$$

that does not affect the dynamics of the system.

IV. THE CHIRAL ANOMALY

A. U(1) anomaly in four dimensions

The chiral transformation on a Dirac field Ψ

$$\delta\Psi(x,t) = -\alpha\gamma^5\Psi(x,t) \tag{4.1}$$

is a symmetry of the equation of motion (3.1). Noether's theorem yields for the γ^5 current

$$(j^5)^\mu(x,t) = \Psi^+(x,t)\gamma^0\gamma^\mu(i\alpha\gamma^5)\Psi(x,t), \tag{4.2}$$

the conservation law

$$\partial_\mu(j^5)^\mu(x,t) = 0. \tag{4.3}$$

To obtain the anomaly of (4.3) we consider the nonconservation of the chiral charge, defined by

$$F^5 = \int_{\Sigma_t}(j^5)^0(x,t)d^3x$$
$$= \sum_{mn}\int_{\Sigma_t}(\varphi_n^t)^+(x)i\alpha\gamma^5\varphi_m^t(x)d^3x c_n^{t+}c_m^t. \tag{4.4}$$

This is precisely the momentum map[17] of the chiral symmetry (4.1) with respect to the symplectic form ω_τ (3.6). To express (4.4) in the holomorphic coordinates (3.17) we note that γ^5 and B_τ commute, so they have a common eigenbase $\{\varphi_n^\tau\}$. With the notion

$$\Phi_{mn}^t := i\int_{\Sigma_t}(\varphi_m^t)^+(x)\alpha\gamma^5\varphi_n^t(x)d^3x, \tag{4.5}$$

we see that these matrix elements Φ_{mn}^t vanish if $\lambda_m^t \neq \lambda_n^t$ and obtain

$$F^5 = \sum_{mn}(z_n^t)^+ z_m^t[(\Phi_{mn}^t)_{\lambda_n^t>0} - (\Phi_{nm}^t)_{\lambda_n^t<0}]. \tag{4.6}$$

This yields the Hamiltonian vector field

$$\xi_{F^5} = +i\sum_{mn}[(\Phi_{mn}^t)_{\lambda_n^t>0} - (\Phi_{nm}^t)_{\lambda_n^t<0}]$$
$$\times\left((z_n^t)^+ \frac{\partial}{\partial(z_m^t)^+} - z_m^t\frac{\partial}{\partial z_n^t}\right). \tag{4.7}$$

As the chiral transformation (4.1) is a symmetry of the theory, the chiral charge (4.4) is conserved under the (classical) Hamiltonian dynamics (3.32):

$$\left.\frac{d}{dt}\right|_{t=\tau} F^5 = \xi_{H_\tau}F^5 + \left.\frac{\partial}{\partial t}\right|_{t=\tau} F^5 = 0. \tag{4.8}$$

Note that the term $\partial/\partial t\, F^5$ occurs due to a possible explicit time dependence via the external field. Quantizing (4.8), i.e., considering the corresponding quantum relation

$$\left.\frac{d}{dt}\right|_{t+\tau}\hat{F}^5 = [\hat{H}_\tau, \hat{F}^5] + \left.\frac{\partial}{\partial t}\right|_{t=\tau}\hat{F}^5, \tag{4.9}$$

with (3.19) we obtain for the prequantum operators (2.24)

$$\mathscr{O}_{H_\tau} = -i\xi_{H_\tau},\quad \mathscr{O}_{F^5} = -i\xi_{F^5}. \tag{4.10}$$

Furthermore, ξ_{F^5} preserves the Kähler polarization provided by $J(t)$ (3.14). So we obtain at $t=\tau$ for a state $|\Sigma\rangle$ given by (3.33)

$$\hat{F}^5|\Sigma\rangle = -i(\xi_{F^5}\mathscr{S})\nu_0 - \tfrac{1}{2}\mathscr{S}[\mathrm{Tr}_{P^\tau}(\mathscr{L}_{\xi_{F^5}})]\cdot\nu_0. \tag{4.11}$$

Fixing $\tau = 0$ for the sequel and using (4.7) we have

$$\langle 0|\hat{F}^5|0\rangle_0 = \langle 0|-i\xi_{F^5}|0\rangle_0$$
$$= -\frac{i}{2}\sum_n\int_{\Sigma_0}(\varphi_n^0)^+(x)$$
$$\times\mathrm{sign}(\lambda_n^0)\alpha\gamma^5\varphi_n^0(x)d^3x. \tag{4.12}$$

Then the anomaly is determined by

$$\mathscr{A} = \left.\frac{d}{dt}\right|_{t=0}\langle 0|\hat{F}^5|0\rangle_t. \tag{4.13}$$

To compute $\langle 0|\hat{F}^5|0\rangle_t$ at $t\neq 0$ we have to use the coordinates provided by (3.30) because of the time-dependent polarization P^t. By the classical conservation law it is clear that the prequantum operators commute ($[\mathscr{O}_{H_\tau}, \mathscr{O}_{F^5}] = 0$) so we obtain

$$\mathscr{A} = \left.\frac{\partial}{\partial t}\right|_{t=0}\sum_n\left(\frac{i}{2}\int_{\Sigma_0}(\varphi_n^0)^+(x)\right.$$
$$\left.\times(\beta_{nm}^{(t,0)})^{-1}\mathrm{sign}(\lambda_m^t)\alpha\gamma^5\beta_{mn}^{(t,0)}\varphi_n^0(x) + \sigma(\delta t)^2\right)$$
$$\simeq \left.\frac{\partial}{\partial t}\right|_{t=0}\sum_n\frac{i}{2}\int_{\Sigma_0}(\varphi_n^0)^+(x)B_t(B_t)^{-1/2}\alpha\gamma^5\varphi_n^0(x). \tag{4.14}$$

Here, $\simeq$ refers to replacing the eigenvalue expression $\mathrm{sign}(\lambda^t) = \lambda^t\cdot(\lambda^t)^{-1/2}$ by the corresponding formal series in the operator B_t. This is an identity in (4.14). However,

the infinite potentially divergent series demands a regularization. Thus we start the summation over the φ_n^0 from small energy eigenvalues λ_n^0, i.e., we choose a regulator

$$\mathscr{R}_0 = \exp\left(-\frac{(\lambda_n^0)^2}{M^2}\right) \simeq \exp\left(-\frac{B_0^2}{M^2}\right), \tag{4.15}$$

and take the limit $M \to \infty$ after the summation:

$$\mathscr{A} = \frac{\partial}{\partial t}\Big|_{t=0} \lim_{M\to\infty} \sum_n \frac{i}{2} \int_{\Sigma_0} d^3x (\varphi_n^0)^+(x) \times iB_t (B_t^2)^{-1/2} \alpha\gamma^5 \mathscr{R}_0 \varphi_n^0(x). \tag{4.16}$$

This expression is well defined and we can proceed in analogy to Ref. 18, changing the basis set to plane waves. We let Tr refer to both the trace over gauge group tr_g and the γ indices tr_γ and define

$$\mathscr{K}^4(x,t) := \lim_{M\to\infty} \mathrm{Tr} \frac{i}{2} \int \frac{d^3k}{(2\pi)^3} e^{+ikx} B_t (B_t^2)^{-1/2} \alpha\gamma^5 \times \exp\left(-\frac{B_0^2}{M^2}\right) e^{-ikz}, \tag{4.17}$$

to obtain

$$\mathscr{A} = \frac{\partial}{\partial t}\Big|_{t=0} \int_{\Sigma_0} d^3x \mathscr{K}^4(x,t). \tag{4.18}$$

To calculate $\mathscr{K}^4(x,t)$ we define the operator

$$B_t(k,x) := \gamma^0\gamma^j \left(k_j + \frac{i\partial_j}{M} + \frac{A_j(x,t)}{M}\right), \tag{4.19}$$

substitute $\mathbf{k} \to \mathbf{k}M$, eliminate the plane wave from the k integral and obtain

$$\mathscr{K}^4(x,t) = \lim_{M\to\infty} \mathrm{Tr}\, M^3 \frac{i}{2} \int \frac{d^3k}{(2\pi)^3} B_t(k,x) (B_t^2(k,x))^{-1/2} \alpha\gamma^5 \times \exp(-B_0^2(k,x)). \tag{4.20}$$

Here, $B_t^2(k,x)$ contains the gauge curvature $F_{jk}(x,t) = i\partial_j A_k - i\partial_k A_j + [A_j, A_k]$:

$$B_t^2(k,x) = \left(k^2 + \frac{2}{M}(\mathbf{k}\mathbf{A}(x,t) + i\mathbf{k}\partial) + \frac{1}{M^2}(2i\mathbf{A}(x,t)\partial + i\partial\mathbf{A} + \mathbf{A}^2 + \partial^2) - \frac{\gamma^j\gamma^k}{2M^2} F_{jk}(x,t)\right). \tag{4.21}$$

Expanding $\mathscr{K}^4(x,t)$ in $(1/M)$ and using results of Eq. (A6), we see that only terms proportional to $\epsilon^{ijk} A_i F_{jk}$ will contribute in the limit $M \to \infty$. Then with (A10) the Taylor expansion yields

$$\begin{aligned}\mathscr{K}^4(x,t) = -2i\epsilon^{ijk}\mathrm{tr}_g \Bigg(&\frac{1}{3}\int \frac{d^3k}{(2\pi)^3} |k| e^{-k^2} \alpha F_{jk}(x,0) A_i(x,0) - \frac{1}{3}\int \frac{d^3k}{(2\pi)^3} \frac{1}{|k|} e^{-k^2} A_i(x,t) \alpha F_{jk}(x,0) \\ &+ \frac{1}{6}\int \frac{d^3k}{(2\pi)^3} \frac{1}{|k|} e^{-k^2} F_{jk}(x,t) \alpha A_i(x,0) - \frac{1}{4}\int \frac{d^3k}{(2\pi)^3} \frac{1}{|k|^3} e^{-k^2} A_i(x,t) F_{jk}(x,t) \alpha \\ &+ \frac{1}{4}\int \frac{d^3k}{(2\pi)^3} \frac{k^2}{|k|^5} e^{-k^2} A_i(x,t) F_{jk}(x,t) \alpha \Bigg).\end{aligned} \tag{4.22}$$

The last two terms are logarithmic divergent but can be properly regulated using (A14). With a cyclic g permutation and the integration (A11) for the convergent terms we have

$$\begin{aligned}\mathscr{K}^4(x,t) = -\alpha \frac{i\epsilon^{ijk}}{12\pi^2} \mathrm{tr}_g \big(&2A_i(x,0) F_{jk}(x,0) \\ &- 2A_i(x,t) F_{jk}(x,0) + A_i(x,0) F_{jk}(x,t) \\ &- A_i(x,t) F_{jk}(x,t)\big),\end{aligned} \tag{4.23}$$

what determines the integrated anomaly to be

$$\begin{aligned}\mathscr{A} &= \frac{i\epsilon^{0ijk}}{4\pi^2} \mathrm{tr}_g \int_{\Sigma_0} d^3x \alpha \dot{A}_i(x,0) F_{jk}(x,0) \\ &= \frac{i\epsilon^{\mu\nu\rho\sigma}}{16\pi^2} \mathrm{tr}_g \int_{\Sigma_0} d^3x \alpha F_{\mu\nu} F_{\rho\sigma}.\end{aligned} \tag{4.24}$$

From the computations it is clear that $\langle 0|F^5|0\rangle_{t=0} = 0$. Furthermore we can repeat the above calculations for the other components of the γ^5 current:

$$\int_{\Sigma_t} (j^5)^k(x,t) d^3x = \sum_{mn} \int_{\Sigma_t} (\varphi_n^t)^+(x) \gamma^0\gamma^k (i\alpha\gamma^5) \varphi_m^t(x) d^3x c_m^+ c_n. \tag{4.25}$$

Using (A2) one can show

$$\left\langle 0 \left| \int_{\Sigma_t} (\hat{j}^5)^k(x,t) d^3x \right| 0 \right\rangle_{t=0} = 0. \tag{4.26}$$

All the calculations hold even if the transformation parameter α in (4.4) is taken to be local, i.e., $\alpha = \alpha(x)$. Choosing $\alpha(x) = \delta(x-y)$ this allows to quantize also the local

relation (4.3) and derive the nonintegrated form of the anomaly, what coincides with the celebrate result (cf. Ref. 8):

$$\partial_\mu \langle 0|(j^5)^\mu(x,t)|0\rangle_{t=0} = (i/16\pi^2)\mathrm{tr}_g \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu} F_{\rho\sigma}. \quad (4.27)$$

B. The chiral U(1) anomaly in D dimensions

To determine the chiral anomaly in D dimensions (D even) we replace γ^5 by $(-(\mathrm{i})^{D/2}\gamma^{D+1})$ and all above considerations naturally generalize from the four-dimensional case. However, to compute

$$\mathscr{K}^D(x,t) = -\lim_{M\to\infty} \mathrm{Tr} \int \frac{d^{D-1}k}{(2\pi)^{D-1}} e^{+ikx} \times B_t (B_t^2)^{-1/2} (i)^{D/2} \alpha \gamma^{D+1} \times \exp(-B_0^2/M^2) e^{ikx}, \quad (4.28)$$

explicitly is a more tedious job. Again we make use of (A6) to argue that in the limit $M\to\infty$ only terms proportional to

$$\epsilon^{ij_1\cdots j_{D-1}} A_i F_{j_1 j_2} \cdots F_{j_{D-2} j_{D-1}} \quad (4.29)$$

will contribute. With the Taylor coefficients of $(1-x)^{-1/2}$ given by

$$b_n = (2n)!/(n!)^2 4^n \quad (4.30)$$

the expansion of (4.28) yields

$$\begin{aligned}\mathscr{K}^D(x,t) = &-(2i)^{D/2}\epsilon\,\mathrm{tr}_g \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \frac{e^{-k^2}}{|k|} \Bigg(\sum_{n=0}^{N} A(x,t) b_n \left(\frac{F(x,t)}{2k^2}\right)^n \alpha \frac{1}{(N-n)!} \left(\frac{F(x,0)}{2}\right)^{N-n} \\ &- \sum_{n=0}^{N} \frac{2b_{n+1}(n+1)}{D-1} A(x,t) \left(\frac{F(x,t)}{2k^2}\right)^n \alpha \frac{1}{(N-n)!} \left(\frac{F(x,0)}{2}\right)^{N-n} \\ &- \sum_{n=0}^{N} b_n \left(\frac{F(x,t)}{2k^2}\right)^n \alpha \frac{2(N-n+1)}{(N-n+1)!} \frac{k^2}{D-1} \left(\frac{F(x,0)}{2}\right)^{N-n} A(x,0) \Bigg). \end{aligned} \quad (4.31)$$

Here we suppressed the indices, set $N := D/2 - 1$, and used (A7). The $n=N$ terms of the first and second sum in (4.31) are infrared divergent and have to be integrated with (A14). The rest is a usual Gauss integral (A11) and yields

$$\begin{aligned}\mathscr{K}^D(x,t) = &-\epsilon \left(\frac{i}{\pi}\right)^{D/2} \mathrm{tr}_g \frac{(D/2-1)!}{(D-1)!} \Big(2b_N A(x,t) (F(x,t))^N \alpha + 2b_N (F(x,t))^N \alpha A(x,0) \\ &+ \sum_{n=0}^{N-1} \left(\frac{D-4-2n}{2}\right)! \frac{b_n (D-1)}{(N-n)!} A(x,t) (F(x,t))^n \alpha (F(x,0))^{N-n} \\ &- \sum_{j=0}^{N-1} \left(\frac{D-4-2n}{2}\right)! \frac{2(n+1)b_{n+1}}{(N-n)!} \alpha(x,t) (F(x,t))^n \alpha (F(x,0))^{N-n} \\ &- \sum_{n=0}^{N-1} \left(\frac{D-2-2n}{2}\right)! \frac{2b_n}{(N-n)!} (F(x,t))^n \alpha (F(x,0))^{N-n} A(x,0) \Big). \end{aligned} \quad (4.32)$$

After a cyclic g permutation this determines the anomaly in D dimensions by

$$\begin{aligned}&\frac{i}{2}\frac{\partial}{\partial t}\Big|_{t=0} \mathscr{K}^D(x,t) \\ &= -i\kappa_D \epsilon^{ij_1\cdots j_{D-1}} \mathrm{tr}_g (\alpha \dot{A}_i(x,0) \\ &\quad \times F_{j_1 j_2}(x,0) \cdots F_{j_{D-2} j_{D-1}}(x,0)), \end{aligned} \quad (4.33)$$

where the coefficient κ_D computes from (4.32) to

$$\kappa_D = \left(\frac{i}{\pi}\right)^{D/2} \frac{(D/2-1)!}{(D-1)!} \left(b_N + \sum_{n=0}^{N-1} b_n\right). \quad (4.34)$$

This induces a recursion formula for κ_D that will be solved by

$$\kappa_D = 2D \left(\frac{i}{4\pi}\right)^{D/2} \frac{1}{(D/2)!}. \quad (4.35)$$

Hence the integrated anomaly in D dimensions is determined by

$$\mathscr{A} = -2 \frac{(i)^{D/2+1} \epsilon^{\mu_0\cdots\mu_{D-1}}}{(D/2)!(4\pi)^{D/2}} \times \int_{\Sigma_0} d^{D-1}x \alpha F_{\mu_0\mu_1} \cdots F_{\mu_{D-2}\mu_{D-1}}. \quad (4.36)$$

C. Non-Abelian anomaly

Also the non-Abelian anomaly[8] can be discussed in this framework. Introducing the pair of orthogonal projection operators

$$\Pi_L=\tfrac{1}{2}(1-i\gamma^5),\ \Pi_R=\tfrac{1}{2}(1+i\gamma^5), \tag{4.37}$$

the space of solutions of the Dirac equation is split into the direct sum $\mathscr{V}=\mathscr{V}_L\oplus\mathscr{V}_R$ of left- and right-handed spinors. Now we consider $\mathscr{V}_L$ to be the space of left-handed solutions only. As Π_L commutes with B_t (because γ^5 does so) we can choose the base $\{\varphi_n\}$ in (3.12) to be given by eigenstates of Π_L. Thus a base of $\mathscr{V}_L$ is provided by the eigenstates to the eigenvalue 1, denoted by $\{\varphi_n^L\}$. The gauge transformation

$$\delta\Psi(x,t)=-i\alpha_a T^a\Psi(x,t), \tag{4.38}$$

yields for the Noether current

$$j^\mu(x,t)=-\Psi^+(x,t)\gamma^0\gamma^\mu(\alpha_a T^a)\Psi(x,t) \tag{4.39}$$

on classical level a covariant conservation law

$$\mathscr{D}_\mu j^\mu(x,t)=0. \tag{4.40}$$

On the quantum level we may obtain the (integrated) non-Abelian anomaly from

$$\mathscr{A}^g=\int(\partial_0\langle 0|\hat{j}^0|0\rangle_t+\langle 0|[\hat{H},\hat{j}^0]|0\rangle_t + [A^i(x,t),\langle 0|\hat{j}^i|0\rangle_t)d^3x. \tag{4.41}$$

The last two terms on the rhs can be shown to vanish at $t=0$. Thus for a theory with left-handed Fermions only we have

$$\mathscr{A}_L^g=\frac{\partial}{\partial t}\Big|_{t=0}\langle 0|\hat{F}_L^g|0\rangle_t, \tag{4.42}$$

where, similar to (4.4),

$$F_L^g=\sum_{\varphi_m,\varphi_n\in\mathscr{V}_L}\mu\left(\int_{\Sigma_0}(\varphi_n^0)^+(x)\alpha_a T^a\gamma^5\varphi_m^0(x)d^3x\right)c_m^+c_n. \tag{4.43}$$

For Π_L eliminates $\mathscr{V}_R$ we can rewrite the summation over $\mathscr{V}_L$ as a sum over all of $\mathscr{V}$ and obtain

$$F_L^{ag}=\sum_{m,n}\left(\int_{\Sigma_0}(\varphi_n^0)^+(x)\alpha_a T^a\Pi_L\varphi_m^0(x)d^3x\right)c_m^+c_n. \tag{4.44}$$

The technical calculation of the anomaly now proceeds in the same way as above. However, the matrix elements Φ_{mn} (4.5) have to be replaced by

$$\Phi_{mn}\to\int_{\Sigma_0}\varphi_m^+(x)\alpha_a T^a\left(\frac{1-i\gamma^5}{2}\right)\varphi_n(x)d^3x. \tag{4.45}$$

Thus we have to compute instead of (4.17)

$$\mathscr{K}^g(x,t)=\lim_{M\to\infty}\mathrm{Tr}\int\frac{d^3k}{(2\pi)^3}e^{+ikx}B_t(B_t^2)^{-1/2}\times\alpha_a T^a\left(\frac{1-i\gamma^5}{2}\right)\exp\left(\frac{-B_0^2}{M^2}\right)e^{-ikx}. \tag{4.46}$$

With B_t^2 from (4.21) and the properties (A2) on the gamma trace we see that only the part containing γ_5 will contribute. After a cyclic g permutation we obtain

$$\mathscr{A}_L^g=\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\,\mathrm{tr}_g\int_{\Sigma_0}d^3x\alpha_a T^a F_{\mu\nu}F_{\rho\sigma}. \tag{4.47}$$

On the other hand the non-Abelian chiral transformation,

$$\delta\Psi(x,t)=-\alpha_a T^a\gamma^5\Psi(x,t), \tag{4.48}$$

can be discussed similarly. For the matrix elements Φ_{mn} we have instead of (4.45)

$$\Phi_{mn}\to\int_{\Sigma_0}\varphi_m^+(x)i\gamma^5\alpha_a T^a\left(\frac{1-i\gamma^5}{2}\right)\varphi_n(x)d^3x, \tag{4.49}$$

and we obtain for the left-handed Fermions

$$\mathscr{A}_L^5=\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\,\mathrm{tr}_g\int_{\Sigma_0}d^3x\alpha_a T^a F_{\mu\nu}F_{\rho\sigma}. \tag{4.50}$$

The same considerations made for a theory with right-handed Fermions only yield

$$\mathscr{A}_R^g=-\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\,\mathrm{tr}_g\int_{\Sigma_0}d^3x\alpha_a T^a F_{\mu\nu}F_{\rho\sigma},$$
$$\mathscr{A}_R^5=\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\,\mathrm{tr}_g\int_{\Sigma_0}d^3x\alpha_a T^a F_{\mu\nu}F_{\rho\sigma}. \tag{4.51}$$

In a theory with different gauge connections A_L and A_R for the left-handed and right-handed Fermions we thus obtain the (covariant) gauge anomaly and the chiral anomaly, respectively, as

$$\mathscr{A}^g=\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\int_{\Sigma_0}d^3x\alpha_a T^a(F_{\mu\nu}[A^L]F_{\rho\sigma}[A^L]-F_{\mu\nu}[A^R]F_{\rho\sigma}[A^R]),$$
$$\mathscr{A}^5=\frac{i\epsilon^{\mu\nu\rho\sigma}}{32\pi^2}\int_{\Sigma_0}d^3x\alpha_a T^a(F_{\mu\nu}[A^L]F_{\rho\sigma}[A^L]+F_{\mu\nu}[A^R]F_{\rho\sigma}[A^R]). \tag{4.52}$$

For the calculation of the consistent anomaly one notes, that the current (4.39) is defined by the gauge transformation (4.38) only up to a constant (in the phase space). Thus the anomaly is determined in our framework only up to the covariant derivative of a (local) polynomial in the gauge field. As shown in Ref. 8 the difference between covariant and consistent anomaly is an expression of this type.

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APPENDIX: TRACES

(1) For the calculations involving γ matrices in D (even) dimensions we use the conventions

$$\{\gamma^\mu,\gamma^\nu\}_+ = 2\eta^{\mu\nu} = 2\,\mathrm{diag}(+,-,\ldots,-),$$
$$(\gamma^\mu)^+ = \gamma^0\gamma^\mu\gamma^0, \tag{A1}$$
$$\gamma^{D+1} = \gamma^0\gamma^1\cdots\gamma^{D-1} \Rightarrow (\gamma^{D+1})^+ = (-)^{D/2-1}\gamma^{D+1}.$$

From this one derives the trace formulas

$$\mathrm{tr}_\gamma(\gamma^{D+1}\gamma^0\gamma^{j_1}\cdots\gamma^{j_k}) = \begin{cases} 0, & k<D-1, \\ 2^{D/2}\epsilon^{j_1,\ldots,j_{D-1}}, & k=D-1, \end{cases}$$
$$\mathrm{tr}_\gamma(\gamma^{D+1}\gamma^{j_1}\cdots\gamma^{j_k}) = 0, \text{ for } 0\notin\{j_1,\ldots,j_k\}, \tag{A2}$$
$$\mathrm{tr}_\gamma(\gamma^0\gamma^{j_1}\cdots\gamma^{j_k}) = 0, \text{ for } 0\notin\{j_1,\ldots,j_k\}.$$

(2) In computing the integral $\mathscr{K}^D(x,t)$ one has not to take care on ultraviolet divergences because of the Gaussian regulator. However, infrared divergences may appear from

$$B_t(B_t^2)^{-1/2} = \frac{\gamma^0\gamma^j}{M}\frac{k_j+D_j}{|k|} \cdot\left(1+\frac{2k_jD_j}{k^2M}+\frac{\gamma^k\gamma^jF_{kl}(x,t)+D_jD_j}{k^2M^2}\right)^{-1/2}, \tag{A3}$$

with $D_j = A_j(x,t) + i\partial_j$. Each term of order $(1/M)^n$ in the expansion of (A3) will contribute with factors $(1/k)^{n-1}$ and $(1/k)^n$. Hence, for the resulting $D-1$ dimensional integral

$$M^{D-1}\int k^{D-2}\,dk\ \mathrm{Polynom}\left(\frac{1}{kM},k\right), \tag{A4}$$

no IR divergences appear in order M^j for $j>0$. In order M^0 there are logarithms divergent contribution and for negative powers of M rational divergences appear, what will be discussed below.

(3) From (A2) it can be seen that in the $1/M$ expansion of $\mathscr{K}^D(x,t)$ only terms will contribute under the γ-trace containing at least $(D-2)/2$ factors

$$(1/M^2)\gamma^j\gamma^kF_{jk}. \tag{A5}$$

On the other hand no more than $(D-1)/2$ such factors can contribute in the limes $M\to\infty$. So performing the γ-trace and suppressing the indices all terms in the expansion will have the form

$$\lim_{M\to\infty}\mathrm{tr}_g M^{D-1}2^{D/2}\epsilon \times\int\frac{d^{D-1}k}{(2\pi)^{D-1}}\frac{e^{-k^2}}{|k|}\mathscr{P}(k^2)\left(-\frac{F}{2M^2}\right)^{D/2-1}\frac{A}{M}, \tag{A6}$$

where $\mathscr{P}(k^2)$ is a Laurent polynom in k^2, determined by the M expansion of $\mathscr{K}^D(x,t)$. Note that one has to take care on the order of terms in (A6), what will be considered below. For computing the polynom $\mathscr{P}$ explicitly we have to replace terms of the form $k_j(\mathbf{kA})$ under the surface integral:

$$\int d^{D-1}kk_i(\mathbf{kA}) = \frac{1}{D-1}\int d^{D-1}kk^2A_i. \tag{A7}$$

(4) Determining $\mathscr{P}(k^2)$ in (A6) one gets from the expansion of $\mathscr{K}^D$ terms of the form

$$\epsilon^{j_1,\ldots,j_n}F_{j_1j_2}(t)\cdots F_{j_{l-1}}(t)\alpha F_{j_{l+1}}(0)\cdots F_{j_{k-1}}(0) \times[i\partial_{j_k}+A_{j_k}(0)]F_{j_{k+1}}(0)\cdots F_{j_{n-1}j_n}(0). \tag{A8}$$

Then we can eliminate the spatial derivative ∂_j from the expression by using

$$\epsilon^{ijk}[i\partial_iF_{jk}(t)] = \epsilon^{ijk}[F_{ij}(t)A_k(t)-A_i(t)F_{jk}(t)], \tag{A9}$$

and shift at $t=0$ the field $A(0)$ to the right. So we get for (A8)

$$\epsilon^{j_1,\ldots,j_n}F_{j_1j_2}(t)\cdots F_{j_{l-2}j_{l-1}}(t) \times\alpha F_{j_{l+1}j_{l+2}}(0)\cdots F_{j_{n-2}j_{n-1}}(0)A_{j_n}(0). \tag{A10a}$$

After integration by parts ∂_{j_l} acts to the left, so we can use the same argument to show

$$\epsilon^{j_1,\ldots,j_n}F_{j_1j_2}(t)\cdots F_{j_{l-1}}(t)[i\partial_{jl}+A_{jl}(t)] \times F_{j_{l+1}}(t)\cdots F_{j_k}(t)\alpha F_{j_{k+1}}(0)\cdots F_{j_n}(0) = \epsilon^{j_1,\ldots,j_n}A_{j_1}(t)F_{j_1j_2}(t)\cdots F_{j_{l-2}j_{l-1}}(t) \times\alpha F_{j_{l+1}j_{l+2}}(0)\cdots F_{j_{n-2}j_{n-1}}(0)A_{j_n}(0). \tag{A10b}$$

(5) The Gaussian integrals in $D-1$ dimensions yield

$$\int\frac{d^{D-1}k}{(2\pi)^{D-1}}|k|^ne^{-k^2} = \left(\frac{1}{\pi}\right)^{D/2}\frac{(D/2-1)!}{2(D-2)!}\left(\frac{D-3+n}{2}\right)!, \tag{A11}$$

for $D-2+n$ positive and odd.

Furthermore, one has to consider the IR divergent integrals

$$\mathscr{I} = \int\frac{e^{-k^2}k^{D-2}dk}{|k|}\left[b_N\left(\frac{1}{k^2}\right)^N - b_{N+1}(N+1)\frac{2(\mathbf{kk})}{D-1}\left(\frac{1}{k^2}\right)^{N+1}\right], \tag{A12}$$

with $N=D/2-1$ [cf. (4.22) and (4.31)]. To regulate the logarithimic divergence we substitute $|k|\to\sqrt{k^2+\epsilon}-\epsilon$ and expand the denominator around $k_\epsilon^2 := k^2+\epsilon$. This yields

$$\mathscr{I} = \sum_j b_N\int e^{-k^2}k^{D-2}c_j^{2N+1}\epsilon^j\left(\frac{1}{k^2+\epsilon}\right)^{N+j+1/2}dk - \frac{2b_{N+1}(N+1)}{D-1}\sum_j\int e^{-k^2}k^Dc_j^{2N+3} \times\epsilon^j\left(\frac{1}{k^2+\epsilon}\right)^{N+j+3/2}dk, \tag{A13}$$

with c_j^{2M+1} the Taylor coefficients of $(\sqrt{1-\epsilon})^{2M+1}$. More rigorously we would have to substitute $k^2\to k^2+M^2\epsilon-M^2\epsilon$ in (4.21) before the expansion of

$B_t^{-1/2}$ in M. By this IR contributions are avoided not only for M^0 but in any order. However, this also yields (A13). Expressing c_j^{2N+3} by c_j^{2N+1} and b_{N+1} by b_N we receive after an integration by parts of the second term of (A13):

$$\mathscr{I}=2b_N\int e^{-k^2}k^D\sum_j\frac{c_j^{2N+1}}{D-1}\epsilon^j\left(\frac{1}{k^2+\epsilon}\right)^{N+j+1/2}dk$$
$$-2\frac{b_N}{D-1}\int e^{-k^2}k^D\frac{1}{k^{D-1}}\,dk=\frac{b_N}{D-1}. \qquad \text{(A14)}$$

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On identically closed forms locally constructed from a field

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Let M be an n-dimensional manifold with derivative operator ∇_a and let $B(M)$ be an arbitrary vector bundle over M, equipped with a connection. A cross section of B defines a field ϕ on M. Let α be a p-form on M (with $p<n$) which is locally constructed from ϕ and finitely many of its derivatives (as well as, possibly, some "background fields" ψ and their derivatives) such that $d\alpha = 0$ for all cross sections ϕ. Suppose further that $\alpha = 0$ for the zero cross section, $\phi = 0$. It is proven here that there exists a $(p-1)$-form β that also is a local function of ϕ,ψ and finitely many of their derivatives, such that $\alpha = d\beta$. A number of applications of this result are described. In particular, gauge invariance is established for the charges and the total fluxes derived from gauge-dependent conserved currents, and severe limitations are established on the the possibilities for gravitational analogs of magnetic charges.

I. INTRODUCTION

In a number of diverse contexts, there arise situations in which one obtains (or seeks to find) a differential p-form α that is locally constructed from a field ϕ and additional, fixed "background fields" ψ such that α is "identically closed," in the sense that $d\alpha = 0$ for all ϕ. (Here, by "fields" ϕ and ψ, we mean sections of a vector bundle. In Sec. II, we will give a precise definition of what we mean by α being "locally constructed" from ϕ and ψ.) By taking the difference between α and its value when $\phi = 0$, we may assume, in addition, that $\alpha = 0$ when $\phi = 0$. In such situations, it is often important to know whether α can be expressed in the form $\alpha = d\beta$, with β a $(p-1)$-form which is similarly locally constructed from ϕ and ψ. The main purpose of this paper is to prove that this is always the case. In this section, we give three examples that illustrate some of the contexts in which the presence of an identically closed form α arises and we explain the relevance of the issue of whether α is of the form $d\beta$, with β locally constructed from ϕ and ψ.

For the first example, we remind the reader that in an arbitrary Lagrangian field theory for a field ξ on an n-dimensional space-time, a symplectic current density[1] ω^μ—or equivalently a symplectic $(n-1)$-form[2] ω—can be constructed in a local manner from a background solution and two "linearized perturbations," $\delta_1\xi, \delta_2\xi$. This form ω satisfies $d\omega = 0$ whenever $\delta_1\xi$ and $\delta_2\xi$ satisfy the linearized field equations. However, in theories with local symmetries, such as the Yang–Mills theory and general relativity, ω fails, in general, to be gauge invariant. One wishes to know whether or not the "charge" $Q \equiv \int_\Sigma \omega$ obtained by integrating ω over a Cauchy hypersurface Σ is gauge invariant. (This is of interest since this charge plays the role of a symplectic form on phase space.[3,1]) To investigate this question, we define $\alpha = \omega(\xi,\delta_1\xi,\delta_2\xi + \delta\xi) - \omega(\xi,\delta_1\xi,\delta_2\xi)$ where $\delta\xi$ denotes the field variation resulting from an arbitrary gauge transformation. We now view ξ, $\delta_1\xi$, $\delta_2\xi$ as "background fields," ψ, and take ϕ to be the (arbitrary) field appearing in the formula for the infinitesimal gauge transformation for $\delta\xi$. Since $\delta\xi$ satisfies the linearized field equations[1] for all ϕ, it follows that α is an identically closed form (for all ϕ), which is locally constructed from ϕ and ψ. If we knew that $\alpha = d\beta$, it would follow immediately that Q is gauge invariant whenever Σ is compact (without boundary). Furthermore, if we knew that β is locally constructed from ϕ and ψ, considerable additional information about the gauge invariance of Q in the noncompact case would be obtained. In the specific cases of the Yang–Mills theory and general relativity, it has been shown[3] by direct, rather laborious calculation, that, indeed, $\alpha = d\beta$ with β locally constructed from ϕ and ψ. Our results proven below show that this property holds quite generally, thus establishing the gauge invariance of Q in a wide variety of contexts without the need for any detailed calculations. Note that similar questions also arise whenever one has a conserved current that is gauge dependent. For example, in the study of vacuum perturbations of a vacuum space-time with Killing field ξ^a, the quantity $j_a = G^{(2)}{}_{ab}\xi^b$ is a conserved, gauge dependent current where $G^{(2)}{}_{ab}$ denotes the second-order Einstein tensor constructed from the perturbation.[4] The results of this paper can be used to establish gauge invariance of the total "gravitational energy flux" defined by j_a when suitable asymptotic conditions are imposed upon the perturbations. In Sec. III we will comment further on the use of our results to prove the gauge invariance of charges and fluxes obtained from gauge dependent conserved currents. As we shall discuss further there, the gauge invariance of Q in the compact case also can be established by alternative arguments; in the noncompact case, however, our theorem yields further useful information.

As a second example of a context in which our basic question arises, we consider the issue of constructing a gravitational analog of "magnetic charge."[5] Here, one seeks a p-form σ, on an n-dimensional manifold M (with $1 \leqslant p \leqslant n-1$) which is locally constructed from a metric g_{ab} and finitely many of its derivatives, and is such that $d\sigma = 0$ for all metrics g_{ab}. The integral of σ over a p-dimensional compact surface which is not homologous to zero would then define a conserved charge. The issue of whether any such nontrivial gravitational charges exist is easily seen to be equivalent to the issue of whether all such identically closed forms σ must be exact. Some partial results on the nonexistence of gravitational charges were previously obtained by direct calculation

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of candidate terms.[5] We shall see in Sec. III that our results can be adapted to prove the following: For Riemannian metrics, any charge obtained from an identically closed form σ must be metric independent (i.e., it must be a topological invariant of M); for Lorentz metrics, any such charge can depend only on the homotopy class (see Finkelstein and Misner[6]) of the metric. Note that our theorem also yields immediate generalizations to cases where additional "background fields" are permitted in the construction of the gravitational charges.

A third illustrative example arose in an investigation[7] of the possible couplings of a spin-two field γ_{ab} to a scalar field ϕ in flat space-time (R^4,η_{ab}). It provides a good illustration of the relevance of the issue of whether α is of the form $d\beta$ with β locally constructed from the fields, as opposed to merely whether α is exact. A possible interaction Lagrangian for γ_{ab} and ϕ is $L_I = \gamma_{ab}\, V^{ab}$, where V^{ab} is an identically conserved (i.e., $\partial_a V^{ab} = 0$) tensor locally constructed from ϕ and η_{ab}. One wishes to know all of the possible candidates for V^{ab}. From the fact that all closed forms are exact (since the topology here is R^4) it is not difficult to show (see problem 5 of Chap. 4 of Ref. 8) that V^{ab} is expressible in the form $V^{ab} = \partial_c\, \partial_d\, V^{acbd}$, where $V^{acbd} = V^{[ac][bd]} = V^{bdac}$. However, it is not clear that V^{ab} can be expressed in this manner using a tensor V^{acbd} which itself is locally constructed from ϕ and η_{ab}. It is of interest to know if this always is the case: If so, then L_I can be reexpressed as a local coupling of the field ϕ to the linearized Riemann tensor of γ_{ab}; if not, then additional possible couplings could arise. It is not difficult to show that this question is equivalent to the question of whether every locally constructed, identically closed form α on R^4 can be expressed as $\alpha = d\beta$ with β locally constructed from ϕ and η_{ab}. Thus the results of this paper eliminate the possibility of any couplings of the above type apart from local couplings of ϕ to the linearized Riemann tensor.

In the next section we shall state and prove our lemmas and theorem. The main task involved in the formulation of these results is to give a precise definition of the notion that the form α is "locally constructed from the fields ϕ and ψ and finitely many of their derivatives." The proof of our results divides into two steps: First, in Lemma 1 a direct proof that $\alpha = d\beta$ with β locally constructed from ϕ and ψ is given for the special case where α depends linearly on ϕ and its derivatives. Then, using this linear result, we give a simple proof for the general case. Some further remarks on the applications of this result are given in Sec. III.

II. FORMULATION AND PROOF OF OUR LEMMAS AND THEOREM

In this section, we shall prove that on an n-dimensional manifold M, any p-form α (with $p < n$) which is locally constructed from fields ϕ and ψ and finitely many of their derivatives and which is closed for all ϕ must be expressible in the form $d\beta$, where the $(p-1)$-form β is similarly locally constructed from ϕ and ψ. As already indicated above, our first main task is to give precise meaning to the notion that the forms α and β are "locally constructed from fields and their derivatives."

To begin we must define what we mean by "fields." Normally, by a field on M one means simply a (smooth) cross section of a fiber bundle, $B(M)$, over M, i.e., a smooth mapping taking each $x \in M$ to the fiber in $B(M)$ over x. However, for our purposes here, it will be convenient to assume that $B(M)$ has the structure of a vector bundle, so here a "field" will mean a cross section of a vector bundle. As discussed at the end of this section, this restriction on $B(M)$ could be eliminated for our main results, but only at the expense of using a more cumbersome notion of derivatives of fields and introducing some further assumptions about $B(M)$. We note that it is not difficult to adapt our arguments and results to typical cases where the fields of interest do not have a natural vector bundle structure. For example, as described in Sec. III, we may treat metrics by viewing them as a sub-bundle of the vector bundle of tensors of type (0,2), then taking into account the fact that α need be defined only on this sub-bundle. As a second example, we may treat the Yang–Mills fields (i.e., connections on a principal fiber bundle) by fixing a connection on the principal bundle and working with the difference between this connection and an arbitrary connection. (This difference has natural vector bundle structure.)

We shall use lower case Greek indices to denote vector space indices for the fibers of $B(M)$, whereas lower case Latin indices will refer to the tangent space of M. Thus a field on M will be denoted as χ^α. As above, we shall use boldface letters to denote differential forms, and, in general, we will suppress the space-time indices on forms.

In order to define derivatives of fields, we shall assume further that $B(M)$ is equipped with a linear connection. In many cases—e.g., if $B(M)$ is a bundle of tensor fields over M and M is equipped with a fixed, background metric—a natural linear connection will be available. If no such connection is available or specified, we simply introduce a fixed linear connection on $B(M)$ in an arbitrary manner. (We may then wish to impose as an additional restriction that the construction of the p-form α be independent of this choice of connection. However, our general framework permits α to depend upon this choice.) Similarly, we also assume that the manifold M is equipped with a fixed affine connection.

In the usual manner, the connection on $B(M)$ allows us to define the derivative of the field χ^α, which may be represented as a tensor field on M with index structure $\nabla_a \chi^\alpha$. It satisfies the standard properties of additivity in χ^α and the Leibnitz rule with respect to multiplication of χ^α by a function $f = M \to \mathsf{R}$. Note that at each $x \in M$, $\nabla_a \chi^\alpha$ arises naturally as a linear map from the tangent space V_x of x in M to the tangent space to the fiber at $\chi(x)$. However, on account of the vector bundle structure assumed for $B(M)$, we may identify the tangent space to the fiber at $\chi(x)$ with the fiber over x, thus allowing us to view $\nabla_a \chi^\alpha$ at $x \in M$ as a linear map from V_x to the fiber over x. This tensor field $\nabla_a \chi^\alpha$ provides the notion we seek of the first derivative of χ^α.

For the purpose of defining second and higher derivatives of χ^α, it is convenient to view $\nabla_a \chi^\alpha$ as a cross section of a new vector bundle $B'(M)$, whose fiber over each $x \in M$ is the tensor product of the fiber of $B(M)$ over x with the cotangent space, $V_x{}^*$, of x in M. The linear connection on $B(M)$ together with the affine connection on M naturally give rise

to a linear connection on this new bundle $B'(M)$. Hence, we may define the second derivative of χ^α—denoted $\nabla_a\nabla_b\chi^\alpha$—as the first derivative of the cross section $\nabla_b\chi^\alpha$ of $B'(M)$. [Note that both the linear connection on $B(M)$ and the affine connection on M are needed to define the second derivative of χ^α, whereas only the linear connection on $B(M)$ was used to define the first derivative.] Continuing in this manner, we obtain the notion of the k th derivative of χ^α as a tensor field with the index structure $\nabla_{a_1}\cdots\nabla_{a_k}\chi^\alpha$. This yields the desired notion of "a field and its derivatives" which we shall use below.

In fact, we wish to allow the p-form α to be considered below to be a function of two types of fields. There will be a "dynamical field" (or fields), denoted ϕ^μ, such that $d\alpha = 0$ for every cross section ϕ^μ, but we also wish to allow for the possibility that α depends upon an additional "background field" (or fields), denoted ψ^ν, and $d\alpha = 0$ (for all ϕ^μ) only for a given, fixed, cross section ψ^ν. (A good example of such a field ψ^ν is a fixed, background metric g_{ab} on space-time.) Thus, we shall assume that the vector bundle $B(M)$ can be expressed as the direct sum of two vector sub-bundles $B_1(M)$ and $B_2(M)$. In order not to introduce any ϕ^μ dependence when we take derivatives of ψ^ν, we shall assume further that the linear connection on $B(M)$ of the previous paragraph arises from linear connections defined separately on $B_1(M)$ and $B_2(M)$. Thus a cross section χ^α of $B(M)$ corresponds to the pair of cross sections (ψ^ν,ϕ^μ) of $B_1(M)$ and $B_2(M)$ respectively, and the derivatives of these cross sections separately—i.e., $\nabla_{a_1}\cdots\nabla_{a_k}\psi^\nu$ and $\nabla_{a_1}\cdots\nabla_{a_k}\phi^\mu$—are well defined.

Note that if we antisymmetrize $\nabla_{a_1}\cdots\nabla_{a_k}\chi^\alpha$ over any pair of cotangent space indices a_i, a_j, the result can be expressed in terms of lower derivatives of χ^α as well as the curvature of both the linear connection on $B(M)$ and the affine connection on M. The curvature of these connections can be treated as a "background field" and incorporated into the field ψ^ν. Thus only the totally symmetric parts $\nabla_{(a_1}\cdots\nabla_{a_k)}\phi^\mu$, of the derivatives of the dynamical field ϕ^μ should be viewed as independent quantities, i.e., all other components of the derivatives of ϕ^μ are determined by the totally symmetrized derivatives together with background fields. Note also that for any point $x\in M$, we can choose a cross section ϕ^μ such that the tensors ϕ^μ, $\nabla_a\phi^\mu,\ldots,\nabla_{(a_1}\cdots\nabla_{a_k)}\phi^\mu$ take on arbitrary prescribed values at x.

We are now ready to define the notion that a p-form α (or other type of tensor field on M) is "locally constructed" from the field χ^α and its first k derivatives. The main aspect of this notion is simply that at each $x\in M$, there is defined a smooth map which takes the tensors χ^α, $\nabla_a\chi^\alpha,\ldots,\nabla_{(a_1}\cdots\nabla_{a_k)}\chi^\alpha$ at x to a p-form α at x. We write this map as $\alpha(\chi^\alpha,\nabla_a\chi^\alpha,\ldots,\nabla_{(a_1}\cdots\nabla_{a_k)}\chi^\alpha)$. [As discussed above, we take α to be a function of only the totally symmetrized derivatives, since only these are independent.] In addition, however, we wish to impose the restriction that α be constructed *solely* out of the quantities of which it is explicitly a function [together with any additional structure specified in the vector bundle $B(M)$], and that for all $x,y\in M$, α is "the same function" of its variables at y as it is of its corresponding variables at x. These further restrictions may be formulated as follows. Given $x,y\in M$, let $L_V:V_x\to V_y$ be a vector space isomorphism between the tangent space V_x to M at x and the tangent space V_y to M at y. Similarly, let $L_F:F_x\to F_y$ be a vector space isomorphism between the fiber F_x over x and the fiber F_y over y. We require further that L_V and L_F preserve any additional structure specified in the fiber bundle. (For example, if the fiber space is given as the direct sum of two subspaces as above, then we require L_F to preserve this direct sum structure. If the fiber at x consists of tensors over V_x, we require L_V and L_F to be such as to preserve this relationship between the fiber space and tangent space.) The maps L_V and L_F induce vector space isomorphisms of arbitrary tensor products of F_x and V_x and their dual spaces $F_x{}^*$ and $V_x{}^*$ with the corresponding tensor product spaces at y. We denote these induced isomorphisms by L^*. Thus L^* maps any tensor at x (with arbitrary Greek and Latin index structure) to a tensor with the same index structure at y. We require that for all allowed L_F and L_V, we have for all cross sections χ^α,

$$L^*\alpha(\chi^\alpha,\nabla_a\chi^\alpha,\ldots,\nabla_{(a_1}\cdots\nabla_{a_k)}\chi^\alpha) = \alpha(L^*\chi^\alpha,L^*\nabla_a\chi^\alpha,\ldots,L^*\nabla_{(a_1}\cdots\nabla_{a_k)}\chi^\alpha), \tag{1}$$

where evaluation of this equation at point y is understood. When $x=y$, this equation expresses the notion that α is constructed solely out of the quantities of which it is explicitly expressed as a function [together with any additional structure specified for $B(M)$], since it is invariant under any isomorphism of F_x and V_x which preserves the fiber bundle structure and leaves these quantities invariant. When $x\neq y$, this equation expresses the notion that α is the same function of its variables at y as it is of its corresponding variables at x.

A differential form α satisfying the properties of the preceding paragraph will be said to be *locally constructed out of the field χ^α and its first k derivatives*. We emphasize that this phrase carries the implication that Eq. (1) is satisfied.

We wish to study p-forms α that are locally constructed out of a field $\chi^\alpha=(\psi^\nu,\phi^\mu)$ and finitely many of its derivatives in the sense defined above, and which have the property that for a given cross section ψ^ν and all cross sections ϕ^μ, we have $d\alpha=0$. To begin we consider the case where α is linear in ϕ^μ and its derivatives. More precisely, we consider α of the general linear form:

$$\alpha_{a_1\cdots a_p} = \sum_{i=0}^{k} A^{(i)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_i}{}_{\mu}\nabla_{(b_1}\cdots\nabla_{b_i)}\phi^\mu. \tag{2}$$

In this equation we have restored the space-time indices for α and, as discussed above, we include only the totally symmetrized derivatives of ϕ^α. Each tensor field $A^{(i)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_i}{}_{\mu}$ occurring in the sum is locally constructed from the background field ψ^ν and its derivatives alone, i.e., it is independent of ϕ^μ. Note, in addition, that we have,

$$A^{(i)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_i}{}_{\mu} = A^{(i)}{}_{[a_1\cdots a_p]}{}^{(b_1\cdots b_i)}{}_{\mu}, \tag{3}$$

where square brackets denote antisymmetrization and, as above, round brackets denote symmetrization.

The following lemma establishes that if such an α is closed for all ϕ^μ, then $\alpha = d\beta$, where β is locally constructed

out of ψ^ν and ϕ^μ. As we shall see, the proof of the corresponding result for the general case (where α is no longer assumed to be linear in ϕ^μ and its derivatives) relies heavily on this lemma.

Lemma 1: Let M be an n-dimensional manifold and let α be a p-form (with $p<n$) of the form (2). Suppose that $d\alpha = 0$ for all cross sections ϕ^μ. Then there exists a $(p-1)$ form β that is locally constructed out of ϕ^μ and the "background field" ψ^ν—and, indeed, β is of the same general form as Eq. (2) except that the upper limit of the sum is $k-1$—such that $\alpha = d\beta$.

Proof: We take the derivative of Eq. (2),

$$\nabla_c \alpha_{a_1\cdots a_p} = \sum_{i=0}^{k} \nabla_c \{A^{(i)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_i}{}_{\mu} \nabla_{(b_1}\cdots\nabla_{b_i)}\phi^\mu\}. \tag{4}$$

By hypothesis, the left side of this equation vanishes when totally antisymmetrized over the indices $c,a_1,\ldots,a_p$. The right side of this equation can be reexpressed as a sum of terms multiplying the totally symmetrized derivatives of ϕ^μ up to order $(k+1)$. Since at each $x\in M$ each of the totally symmetrized derivatives of ϕ^μ may be specified independently, each of these terms must vanish separately when antisymmetrized over $a_1,\ldots,a_p,c$. We focus attention on the highest derivative term:

$$\zeta_{a_1\cdots a_p c} \equiv A^{(k)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{\mu} \nabla_{(c}\nabla_{b_1}\cdots\nabla_{b_k)}\phi^\mu. \tag{5}$$

Then, we have,

$$\zeta_{[a_1\cdots a_p c]} = 0. \tag{6}$$

We may write Eq. (6) in the form,

$$A^{(k)}{}_{[a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{|\mu|}\delta^d{}_{c]}\nabla_{(d}\nabla_{b_1}\cdots\nabla_{b_k)}\phi^\mu = 0, \tag{7}$$

where $\delta^d{}_c$ denotes the identity map. However, since, at any $x\in M$, $\nabla_{(d}\nabla_{b_1}\cdots\nabla_{b_k)}\phi^\mu$ can be chosen to be an arbitrary totally symmetric tensor, Eq. (7) will hold for all cross sections ϕ^μ if and only if we have,

$$A^{(k)}{}_{[a_1\cdots a_p}{}^{(b_1\cdots b_k}{}_{|\mu|}\delta^{d)}{}_{c]} = 0. \tag{8}$$

We now contract Eq. (8) over the indicies c and d. When all of the terms resulting from the symmetrization and antisymmetrization are written out, the index d will appear on the tensor $\delta^b{}_a$ a fraction $1/(k+1)$ of the time, and the index c will appear on $\delta^b{}_a$ a fraction $1(p+1)$ of the time. Taking this into account, we obtain,

$$\left[\frac{n}{(k+1)(p+1)}+\frac{k}{(k+1)(p+1)}-\frac{p}{(k+1)(p+1)}\right]A^{(k)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{\mu}$$
$$-\frac{kp}{(k+1)(p+1)}A^{(k)}{}_{c[a_2\cdots a_p}{}^{c(b_2\cdots b_k}{}_{\mu}\delta^{b_1)}{}_{a_1]} = 0, \tag{9}$$

where the symmetries of $A^{(k)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{\mu}$ [see Eq. (3)] have been used. Thus we have shown that if α is identically closed, the coefficient $A^{(k)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{\mu}$, of the highest derivative term in the expression (2) for α must satisfy,

$$A^{(k)}{}_{a_1\cdots a_p}{}^{b_1\cdots b_k}{}_{\mu} = \frac{kp}{n-p+k}A^{(k)}{}_{c[a_2\cdots a_p}{}^{c(b_2\cdots b_k}{}_{|\mu|}\delta^{b_1)}{}_{a_1]}. \tag{10}$$

We now prove our result by induction on the highest number of derivatives, k, of ϕ^μ appearing in Eq. (2). For the case $k=0$, Eq. (10) simply reduces to,

$$A^{(0)}{}_{a_1\cdots a_p\mu} = 0, \tag{11}$$

i.e., there are no nontrivial, identically closed, locally constructed p-forms that depend linearly only upon ϕ^μ and not upon its derivatives. Choosing $\beta = 0$, we see that our lemma holds for the case $k=0$.

Now, let $k = m \geqslant 1$ and assume that the lemma holds for all $k<m$. Define the $(p-1)$ form τ by,

$$\tau_{a_2\cdots a_p} = \frac{m}{n-p+m}A^{(m)}{}_{ca_2\cdots a_p}{}^{cb_2\cdots b_m}{}_{\mu}\nabla_{b_2}\cdots\nabla_{b_m}\phi^\mu. \tag{12}$$

Then τ is manifestly locally constructed from ψ^ν, ϕ^μ, and their derivatives, and, indeed, it is linear in the $(m-1)$st derivative of ϕ^μ. Most importantly, it follows directly from Eq. (10) that α and $d\tau$ have precisely the same coefficient of the mth symmetrized derivative of ϕ^μ. Now, let

$$\alpha' = \alpha - d\tau. \tag{13}$$

Then, α' is locally constructed from ψ^ν and ϕ^μ, is linear in ϕ^μ, is closed for all ϕ^μ, but α' depends only on derivatives of ϕ^μ only up to order $(m-1)$. Hence, by the inductive hypothesis, we have $\alpha' = d\rho$ for some ρ locally constructed from ψ^ν and ϕ^μ, and their derivatives. Furthermore, ρ is of the general form (2), with the upper limit of the sum now extending to $m-2$. Thus setting

$$\beta = \tau + \rho, \tag{14}$$

we obtain the desired result. □

Note that this lemma not only establishes existence of the $(p-1)$-form β but it also gives an explicit constructive procedure for finding β: One simply writes α in the form (2) and defines the first contribution τ to β by Eq. (12). Then one subtracts $d\tau$ from α and repeats this procedure until α is reduced to zero. As already noted in the lemma, the β constructed by this means is linear in ϕ^μ and its derivatives and depends upon derivatives of ϕ^μ only up to order $k-1$ [where k is the number of derivatives of ϕ^μ appearing in the original expression (2) for α]. However, it should be noted that if α depends upon derivatives of ψ^ν up to order s, then β may depend upon derivatives of ψ^ν as high as order $s+k-1$, since each subtraction of a term of the form "$d\tau$" in the procedure may introduce an additional derivative of ψ^ν.

Unfortunately, the direct proof given in the lemma does not appear to have an easy generalization even to the next simplest case where α is a quadratic (rather than linear) function of ϕ^μ and its derivatives. Remarkably, however, a simple proof for the general case can be obtained directly from the following lemma, which is essentially a corollary to the proceeding lemma. As we shall see in an application given at the end of Sec. III, this lemma is quite useful in its own right.

Lemma 2: Let M be an n-dimensional manifold and let α be a p-form (with $p<n$) which is locally constructed out of the fields ψ^ν, ϕ^μ, and their derivatives in the sense explained above, so that

$$\alpha = \alpha(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_s)} \psi^\nu; \phi^\mu, \nabla_a \phi^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_k)} \phi^\mu). \tag{15}$$

Suppose further that $d\alpha = 0$ for all cross sections ϕ^μ. Let $\phi^\mu(\lambda)$ denote an arbitrary, smooth one-parameter family of cross sections and write

$$\dot{\alpha} \equiv \frac{d\alpha}{d\lambda}. \tag{16}$$

Then there exists a $(p-1)$ form γ that is locally constructed from the fields ψ^ν, ϕ^μ, and $\dot{\phi}^\mu \equiv d\phi^\mu/d\lambda$ and their derivatives, i.e.,

$$\gamma = \gamma(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_q)} \psi^\nu; \phi^\mu, \nabla_a \phi^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_r)} \phi^\mu; \dot{\phi}^\mu, \nabla_a \dot{\phi}^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_{k-1})} \dot{\phi}^\mu), \tag{17}$$

such that for the given ψ^ν and for every one-parameter family $\phi^\mu(\lambda)$ we have at each λ,

$$\dot{\alpha} = d\gamma. \tag{18}$$

Proof: We calculate $\dot{\alpha}$ using the chain rule. Since ψ^ν is λ independent we obtain contributions only from the dependence of α on ϕ^μ and its derivatives, so the resulting expression is linear in $\dot{\phi}^\mu$ and its derivatives up to order k. We now view $\dot{\alpha}$ as a p form that is locally constructed from ψ^ν, ϕ^μ, $\dot{\phi}^\mu$, and their derivatives, where we view these three fields as independent. Since α is defined for all cross sections ϕ^μ and hence all one-parameter families $\phi^\mu(\lambda)$, it follows that $\dot{\alpha}$ is defined for all ϕ^μ and $\dot{\phi}^\mu$. Furthermore, since differentiation with respect to λ commutes with exterior differentiation, we have,

$$d\dot{\alpha} = 0, \tag{19}$$

for all $\dot{\phi}^\mu$ (as well as for all ϕ^μ). Thus $\dot{\alpha}$ satisfies all the hypotheses of lemma 1, with the role of ψ^ν in that lemma now being played by ψ^ν and ϕ^μ, and the role of ϕ^μ now being played by $\dot{\phi}^\mu$. The desired conclusion now follows immediately from that lemma. □

Note that if α depends upon derivatives of ϕ^μ up to order k, then by Lemma 1, γ may depend upon derivatives of $\dot{\phi}^\mu$ up to at most order $k-1$, as already indicated in Eq. (17). However, by the remark below Lemma 1, γ may depend upon derivatives of ϕ^μ as high as order $r = 2k-1$.

We now state and prove our principal result.

Theorem: Let M be an n-dimensional manifold and let α be a p-form (with $p < n$) which is locally constructed out of the fields ψ^ν, ϕ^μ, and their derivatives and is such that $d\alpha = 0$ for all cross sections ϕ^μ. Suppose further that $\alpha = 0$ for the zero cross section $\phi^\mu \equiv 0$. Then there exists a $(p-1)$-form β which is locally constructed from ψ^ν, ϕ^μ and their derivatives such that $\alpha = d\beta$.

Proof: By Lemma 2, we know that there exists a $(p-1)$-form γ of the form (17) such that Eq. (18) holds for all one-parameter families $\phi^\mu(\lambda)$. We apply this result to the family

$$\phi^\mu(\lambda) = \lambda \phi^\mu, \tag{20}$$

where ϕ^μ is an arbitrary cross section. We thereby obtain,

$$\dot{\alpha}(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_s)} \psi^\nu; \lambda\phi^\mu, \lambda\nabla_a \phi^\mu, \ldots, \lambda\nabla_{(a_1} \ldots \nabla_{a_k)} \phi^\mu) = d\gamma(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_q)} \psi^\nu; \lambda\phi^\mu, \lambda\nabla_a \phi^\mu, \ldots, \lambda\nabla_{(a_1} \cdots \nabla_{a_r)} \phi^\mu; \phi^\mu, \nabla_a \phi^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_{k-1})} \phi^\mu), \tag{21}$$

where we have substituted the values $\phi^\mu(\lambda) = \lambda\phi^\mu$ and $\dot{\phi}^\mu = \phi^\mu$ in Eqs. (17) and (18). Now we simply integrate Eq. (21) over λ from 0 to 1. Using the fact that $\alpha = 0$ when $\phi^\mu \equiv 0$, we find that the left side yields α evaluated for the fields ψ^ν, ϕ^μ. To express the right side in the desired form, we define the $(p-1)$-form β by

$$\beta(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_s)} \psi^\nu; \phi^\mu, \nabla_a \phi^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_r)} \phi^\mu) = \int_0^1 d\lambda\, \gamma(\psi^\nu, \nabla_a \psi^\nu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_q)} \psi^\nu; \lambda\phi^\mu, \lambda\nabla_a \phi^\mu, \ldots, \lambda\nabla_{(a_1} \cdots \nabla_{a_r)} \phi^\mu; \phi^\mu, \nabla_a \phi^\mu, \ldots, \nabla_{(a_1} \cdots \nabla_{a_{k-1})} \phi^\mu) \tag{22}$$

Then β is locally constructed out of the fields ψ^ν, ϕ^μ and their derivatives. Since exterior differentiation commutes with integration with respect to λ, we obtain,

$$\alpha = d\beta \tag{23}$$

as we desired to show. □

Note that the proof of our theorem also gives a constructive procedure for obtaining β in the general case. We simply linearize α about an arbitrary field configuration ϕ^μ and apply the constructive procedure of Lemma 1 to $\dot{\alpha}$ to obtain γ. Then we obtain β by performing the integral (22). Note that by the remark below lemma 2, β may depend upon derivatives of ϕ^μ up to order $r = 2k-1$, even though α depends upon the derivatives of ϕ^μ only up to order k.

Finally, we comment upon the extent to which vector bundle structure for the fields ψ^ν, ϕ^μ is needed for our results. There are three main places above where we made use of vector bundle structure. First, we used a linear connection (defined only for vector bundles) to define the notion of derivatives of fields used in the formulation of our lemmas and theorem. However, as indicated at the beginning of this section, this use of vector bundle structure is not essential, i.e., one could formulate a suitable notion of derivatives of fields in the absence of vector space structure for the fibers. Second, Lemma 1 is formulated for the case where α is linear in ϕ^μ and its derivatives, a notion that makes sense only when vector bundle structure is present. Thus vector bundle structure clearly is essential for Lemma 1. However, the application of Lemma 1 to the proof of Lemma 2 uses this vector bundle structure in an essential way only with respect to the

"linearized field" $\dot{\phi}^\mu$. Such a linear structure for $\dot{\phi}^\mu$ is always naturally present (even if the field ϕ^μ fails to have vector bundle structure), so the assumption of vector bundle structure for ψ^ν and ϕ^μ is not essential for the formulation and proof of Lemma 2. Finally, vector bundle structure for ϕ^μ was used to define the general prescription (20) for the one-parameter family used in the proof of the theorem. This family satisfies two key properties: (i) It provides a homotopy of any cross section ϕ^μ to a given, fixed cross section (in this case, the zero cross section). (ii) It is entirely "local" in character in that $\phi^\mu(\lambda)$ and its derivatives at point $x \in M$ depend only upon the corresponding value and derivatives of the original cross section ϕ^μ at x. Both of these properties play an essential role in the proof of the theorem. [If property (ii) did not hold, we would be unable to write down a formula like Eq. (22) that defines β as a local function of ϕ^μ and its derivatives.] Thus for our theorem, in order to eliminate the assumption of vector bundle structure for the field ϕ^μ, it would be necessary to introduce additional assumptions that would ensure existence of a one-parameter family satisfying these two properties.

III. SOME APPLICATIONS

Several representative applications of the theorem of the previous section were already mentioned in Sec. I. In this section, we will discuss some further aspects of the first two of these applications.

Recall that the first application was to the proof of the gauge invariance of a charge Q associated with a gauge dependent but identically closed (i.e., closed in all gauges) p-form ω. Here, it is assumed that the gauge transformations are generated by an arbitrary cross section, ϕ^μ, of a vector bundle. In the case where the charge is obtained by integrating over a compact boundaryless surface Σ the theorem of the previous section directly implies

$$Q[\phi^\mu] - Q[0] = \int_\Sigma \{\omega[\phi^\mu] - \omega[0]\} = \int_\Sigma \alpha = \int_\Sigma d\beta = 0, \tag{24}$$

thus giving a very simple proof of the gauge invariance of Q.

It is worth noting, however, that when Σ is compact the gauge invariance of Q also can be proven (at least in certain cases) in the following manner.[9] Consider, first, the case where Σ can be deformed in M to a disjoint surface Σ' such that $\Sigma \cup \Sigma'$ comprises the boundary of a compact region. We wish to show that for any ϕ^μ, we have $Q[\phi^\mu] = Q[0]$, where $Q \equiv \int_\Sigma \omega$. To do so, we define the charge $Q' \equiv \int_{\Sigma'} \omega$ associated with the "deformed surface" Σ' and choose an "interpolating field" $\tilde{\phi}^\mu$ so that $\tilde{\phi}^\mu = \phi^\mu$ in a neighborhood of Σ but $\tilde{\phi}^\mu = 0$ in a neighborhood of Σ'. Since $\omega[\tilde{\phi}^\mu]$ is closed, we have

$$Q'[\tilde{\phi}^\mu] = \int_{\Sigma'} \omega[\tilde{\phi}^\mu] = \int_\Sigma \omega[\tilde{\phi}^\mu] = Q[\tilde{\phi}^\mu]. \tag{25}$$

However, since ω is locally constructed from the fields upon which it depends, we clearly have

$$Q'[\tilde{\phi}^\mu] = Q'[0] \text{ and } Q[\tilde{\phi}^\mu] = Q[\phi^\mu]. \tag{26}$$

Finally, since $\omega[0]$ also is closed, we have

$$Q'[0] = Q[0]. \tag{27}$$

Equations (25)–(27) prove the desired result,

$$Q[\phi^\mu] = Q[0], \tag{28}$$

for the case we have been considering, namely, where Σ and Σ' are disjoint and $\Sigma \cup \Sigma'$ comprises the boundary of a compact region. In some cases, however, it may be impossible to deform Σ to a surface Σ' that does not intersect Σ. Nevertheless, it still should be possible to prove the gauge invariance of Q by applying the above type of argument to successive deformations of Σ, where the intersection points are varied in the successive deformations.

Although the above argument succeeds in proving the gauge invariance of Q for compact Σ (at least when a Σ' can be chosen disjoint from Σ) without appealing to our theorem, for the case of noncompact Σ the analysis of the gauge invariance of Q using our theorem can have a definite advantage over the corresponding analysis using the above type of argument. Namely, to treat the noncompact case by means of our theorem, we let $\partial\Sigma$ bound a compact region of Σ, and then take the limit as $\partial\Sigma$ "goes to infinity." If $\int_{\partial\Sigma} \beta \to 0$ in this limit for all allowed ϕ^μ, then it follows from Eq. (24) that Q will be gauge invariant; if not, Q will be gauge dependent. Even if one does not employ the constructive procedure described in the previous section to obtain an explicit formula for β, it often will be possible to prove gauge invariance (for the given asymptotic conditions on the fields) by using the fact that β is locally constructed from the fields and their derivatives together with some knowledge of the kinds of terms that can appear in β. By contrast, if the alternative argument is used, one must analyze the asymptotic behavior of α for an "interpolating field" $\tilde{\phi}^\mu$ over a surface joining $\partial\Sigma$ to $\partial\Sigma'$, and it is likely to be more difficult to obtain as sharp a criterion for the gauge invariance of Q.

We turn now to the second application discussed in Sec. I, namely, to the issue of obtaining an analog of magnetic charge for metrics, i.e., an identically closed (but not always exact) p-form σ (with $p < n$) which is defined for all metrics (of a given signature) and is locally constructed from the metric and its derivatives. We discuss that application further here since it provides a good illustration of how the results of Sec. II can be applied in a case where the fields under consideration do not possess a natural vector bundle structure.

The metrics of a given signature on a manifold M are, of course, a sub-bundle of the vector bundle of tensor fields of type (0,2). However, the fibers of this sub-bundle do not have a natural vector space structure, and σ is defined only for cross sections of this sub-bundle. In particular, the zero cross section does not define a metric, so σ will not be defined for the one-parameter family, Eq. (20), used in the proof of the theorem. However, this difficulty is easily remedied for the case of Riemannian metrics, since the Riemannian metrics at any point $x \in M$ comprise a convex subset of the tensors of type (0,2) at x. Hence, we can simply fix an (arbitrarily chosen) Riemannian metric ${g^{(0)}}_{ab}$ and instead consider the one-parameter family $g_{ab}(\lambda) = \lambda g_{ab} + (1-\lambda){g^{(0)}}_{ab}$ for $\lambda \in [0,1]$. Each member of this family is a Riemannian metric. When applied to this family, the proof of the theorem of

the previous section now yields the result that $\sigma[g_{ab}] - \sigma[g^{(0)}{}_{ab}]$ is of the form $d\beta$, where β is locally constructed from g_{ab} and $g^{(0)}{}_{ab}$ and their derivatives. In particular, this implies that the "charge" Q obtained by integrating σ over a p-dimensional compact surface must be metric independent, i.e., for all g_{ab} we have, $Q[g_{ab}] = Q[g^{(0)}{}_{ab}]$.

The situation is somewhat more interesting for the case of Lorentzian metrics, which do not comprise a convex set. We can obtain some (fairly weak) results by applying the argument of the previous paragraph to certain convex subsets of Lorentz metrics, e.g., those which possess a fixed timelike covector w_a in common. However, for the issue at hand, a much stronger result can be obtained by appealing to Lemma 2 rather than the theorem of the previous section. (As mentioned at the end of Sec. II, vector bundle structure is not needed for Lemma 2.) Consider two Lorentz metrics, $g^{(0)}{}_{ab}$ and $g^{(1)}{}_{ab}$, which in a neighborhood of Σ can be joined by a smooth homotopy of Lorentz metrics $g_{ab}(\lambda)$. Let $Q(\lambda)$ be the charge of $\sigma[g_{ab}(\lambda)]$ for the compact surface Σ, i.e., $Q(\lambda) = \int_\Sigma \sigma[g_{ab}(\lambda)]$. Then, according to Lemma 2, we have,

$$\frac{dQ}{d\lambda} = \int_\Sigma \dot{\sigma} = \int_\Sigma d\gamma = 0, \tag{29}$$

which immediately implies that $Q[g^{(0)}{}_{ab}] = Q[g^{(1)}{}_{ab}]$, that is, Q can depend only upon the homotopy class of the metric. Note that while this argument also implies that $\sigma[g^{(1)}{}_{ab}] - \sigma[g^{(0)}{}_{ab}]$ is exact, it does not imply that it can be expressed in the form $d\beta$, with β locally constructed from $g^{(1)}{}_{ab}$, $g^{(0)}{}_{ab}$, and their derivatives.

The fact that any gravitational analog of magnetic charge must be metric independent in the case of Riemannian metrics and must depend only upon the homotopy class in the Lorentzian case puts strong restrictions upon any candidate expression for σ. For example, from merely the invariance of Q under a constant scale transformation of the metric, $g_{ab} \to kg_{ab}$, it follows that any identically closed p-form σ which is a polynomial in g_{ab}, g^{ab}, the curvature of g_{ab}, and the covariant derivatives of the curvature must have degree[5] $N = p$ if it is to have a possibility of yielding a nonidentically vanishing charge. (Here, N is defined as $2r + q$, where r is the total number of curvature tensors and q is the total number of covariant derivatives in each term.) Since Unruh[5] has explicitly ruled out all candidate polynomials with $N \leqslant 5$ for Lorentz metrics in four dimensions and only the case $p \leqslant 3$ is relevant in that case, it follows that no polynomial expression for a gravitational charge exists for 4-dimensional space-times. The k th Pontrijagin class (see, e.g., Ref. 10) provides an identically closed $4k$-form that is polynomial in the curvature, thus providing nontrivial gravitational charges in dimensions greater than four. It seems possible that the Pontrijagin classes provide the only nontrivial examples of gravitational charges, but an analysis of whether this is the case is left for future investigations.

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Schrödinger processes and large deviations

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For a large system of independent diffusing particles, each of which is killed at a certain space-time dependent rate, the conditional distribution of surviving trajectories in a bounded time interval is computed, given the approximate form of the initial and final empirical distribution of surviving particles. This generalizes a result for the Brownian case without killing, which was first obtained by Schrödinger [Sitzungsber. Preuss. Akad. Wiss. Phys. Math. Kl. **1931**, 144].

I. INTRODUCTION

Let $p(s,x;t,y)$ be the fundamental solution of the heat equation $(\partial/\partial s + \frac{1}{2}\Delta + c)p = 0$, where $c = c(s,x)$ is a bounded, continuous scalar field satisfying a Hölder condition with respect to x on $[0,T]\times\mathbf{R}^d$ (these conditions actually guarantee the existence of p on $[0,T]$, cf. Friedman,[1] p. 23). Consider a probability measure Q^* on path space $\Omega = C([0,T],\mathbf{R}^d)$, whose finite-dimensional distributions are of the form [where (X_t) denotes, here and throughout, the canonical process on Ω]

$$Q^*[X_0\in dx, X_{t_1}\in dy_1,\ldots,X_{t_n}\in dy_n, X_T\in dz]$$
$$= p(0,x;t_1,y_1)\cdots p(t_n,y_n;T,z)\mu_0(dx)dy_1\cdots dy_n\mu_T(dz)$$

for some measures μ_0, μ_T on $\mathbf{R}^d$. It turns out that Q^* is Markovian; in fact, as proved by Jamison,[2] it is the only Markovian among all "reciprocal" (i.e., two-sided Markov) distributions Q with two-sided transition density

$$[1/p(s,x;u,z)]p(s,x;t,\cdot)p(t,\cdot;u,z)$$

and with the same initial and final distribution as Q^*.

In the case $c = 0$, Schrödinger[3] showed that Q^* yields the most likely "intermediate" (one-time) distributions for a large number of independent and identically distributed (i.i.d.) particles with given (or measured) initial and final empirical distributions. Föllmer[4] gives a modern and rigorous proof of this result in terms of large deviations. Consistent with Jamison[5] and Föllmer[4] and following Nagasawa[6] we will call Q^* a *Schrödinger process* or *Schrödinger bridge* also in case of nonvanishing c.

Wakolbinger[7] showed that among all not necessarily Markovian diffusion processes with drift (β_t), diffusion constant one, and prescribed initial and final distributions, Schrödinger's process minimizes the action functional

$$E\left[\int_0^T \left(\frac{1}{2}\beta_t^2 - c(t,X_t)\right)dt\right].$$

Related variational characterizations have been obtained by Nagasawa,[8] Zambrini,[9] Cruzeiro and Zambrini,[10] Blanchard *et al.*,[11] Kime and Blaquiere,[12] Dai Pra and Pavon;[13] see also the references given there. In the present paper we give an extension of the Schrödinger–Föllmer result to the case of nonvanishing c.

Consider a large number of i.i.d diffusing particles, each being killed independently with rate $M - c(s,x)$, where the constant M is some upper bound of c. Then Schrödinger's process yields the most likely distribution of surviving trajectories, given the initial and final distribution of surviving particles. (The case $c = 0$, $M = 0$ corresponds to Schrödinger's result.)

II. SCHRÖDINGER BRIDGES

The basic object will be a strictly positive transition density $p(s,x;t,y)$ obeying the Chapman–Kolmogorov equations

$$\int p(s,x;t,y)p(t,y;u,z)dy = p(s,x;u,z)$$
$$\text{for all } x,z\in\mathbf{R}^d, 0\leqslant s<t<u<T, \tag{1}$$

but not necessarily obeying

$$\int p(s,x;t,y)dy = 1. \tag{2}$$

Equation (1) implies that for all $x,z\in\mathbf{R}^d$:

$$[1/p(0,x;T,z)]p(0,x;t_1,y_1)p(t_1,y_1;t_2,y_2)$$
$$\cdots p(t_n,y_n;T,z)dy_1\cdots dy_n \tag{3}$$

defines a consistent system of probability measures. We will assume that for all $x,z\in\mathbf{R}^d$ there exists a probability distribution P_x^z on $\Omega := C([0,T];\mathbf{R}^d)$ having (3) as its finite-dimensional distributions and obeying $P_x^z[X_0 = x, X_T = z] = 1$.

Definition 1: Any probability measure P on Ω which is of the form

$$P = \int P_x^z \nu(dx,dz)$$

for some probability measure ν on $\mathbf{R}^d\times\mathbf{R}^d$ will be called a *p bridge*.

[In the terminology of Jamison[2] (resp. Zambrini[9]), (X_t,P) is a *reciprocal* (resp. *Bernstein*) *process* with reciprocal (resp. Bernstein) transition density $[1/p(s,x;u,z)]p(s,x;t,\cdot)p(t,\cdot;u,z)$.]

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Proposition 1 (Jamison,[2] Theorem 3.1, Zambrini,[9] Theorem 3.3): A p bridge Q is Markovian if and only if it is of the form

$$Q = \int P^z_x \mu_0(dx) p(0,x;T,z) \mu_T(dz) \tag{4}$$

for some measures μ_0, μ_T on $\mathbf{R}^d$.

Definition 2: A Markovian p bridge Q with marginals $Q[X_0 \in \cdot\,] = \nu_0$, $Q[X_T \in \cdot\,] = \nu_T$ will be called a Schrödinger process (or Schrödinger bridge) specified by p, ν_0, and ν_T.

Remark: Projection of (4) to times 0 and T, respectively, yields the so-called Schrödinger system:

$$\begin{aligned} \nu_0(dx) &= \mu_0(dx) \int \mu_T(dz) p(0,x;T,z), \\ \nu_T(dz) &= \mu_T(dz) \int \mu_0(dx) p(0,x;T,z), \end{aligned} \tag{5}$$

where ν_0, ν_T are the initial and final distributions of the Markovian p bridge Q. Hence, for any given ν_0, ν_T, obviously the following assertions are equivalent: (i) There exists a unique Schrödinger bridge specified by p, ν_0, and ν_T. (ii) There exists a solution μ_0, μ_T of the Schrödinger system (5), and all its solutions are of the form $c\mu_0$, $(1/c)\mu_T$, $c > 0$. Jamison[2] shows that, for any choice of ν_0, ν_T, (ii) holds under the assumption that $p(0,\cdot;T,\cdot)$ is continuous.

III. SCHRÖDINGER BRIDGES AND MINIMAL ENTROPY

Let σ be a fixed probability measure on $\mathbf{R}^d$; assume that

$$k := \int \sigma(dx) p(0,x;T,z) dz < \infty. \tag{6}$$

Put $\mu(dx,dz) := \sigma(dx)p(0,x;T,z)dz$ and $P := \int P^z_x \mu(dx, dz)$; note that assumption (6) implies that P is a finite measure on Ω with total mass $P(\Omega) = \mu(\mathbf{R}^d \times \mathbf{R}^d) = k$. We put $\tilde{P} := [1/P(\Omega)]P$, and recall that, for any two probability distributions Q_1, Q_2 on Ω, the relative entropy of Q_1 with respect to Q_2 is defined by

$$H(Q_1,Q_2) := \int \left(\ln \frac{dQ_1}{dQ_2} \right) dQ_1$$

[where $H(Q_1,Q_2) := \infty$ if Q_1 is not absolutely continuous with respect to Q_2].

Proposition 2: Let ν_0, ν_T be given probability measures on $\mathbf{R}^d$.

The following are equivalent. There exists some probability measure ν on $\mathbf{R}^d \times \mathbf{R}^d$ with marginals ν_0, ν_T and

$$\int \left(\ln \frac{d\nu}{d\mu} \right) d\nu < \infty. \tag{7}$$

There exists some probability measure Q on Ω with marginals

$$Q[X_0 \in \cdot\,] = \nu_0, \quad Q[X_T \in \cdot\,] = \nu_T, \text{ and } H(Q,\tilde{P}) < \infty. \tag{8}$$

In this case [i.e., if (7) and (8) hold], the minimization problem $H(Q,\tilde{P})$ = minimum over the probability measures Q on Ω with marginals

$$Q[X_0 \in \cdot\,] = \nu_0, \quad Q[X_T \in \cdot\,] = \nu_T$$

has a unique solution Q^*, and Q^* is a Schrödinger bridge specified by p, ν_0 and ν_T.

Proof: (1) Let ν be as in (7), and put

$$Q := \int P^z_x \nu(dx,dz).$$

Since

$$\tilde{P} = \frac{1}{k} \int P^z_x \mu(dx,dz),$$

we get

$$\frac{dQ}{d\tilde{P}}(X) = k \frac{d\nu}{d\mu}(X_0,X_T) \quad Q\text{-a.s.},$$

which shows that Q obeys (8).

(2) Conversely, let Q be as in (8), put $\nu(dx,dz) := Q[X_0 \in dx, X_T \in dz]$, and denote the disintegration of Q with respect to (X_0,X_T) by (Q^z_x). Since

$$H(Q,\tilde{P}) = \int \left(\ln \frac{d\nu}{d\mu/k} \right) d\nu + \int \left(\ln \frac{dQ^z_x}{dP^z_x} \right) dQ^z_x \nu(dx,dz), \tag{9}$$

and since by assumption $H(Q,\tilde{P}) < \infty$, and, moreover, the relative entropy is always non-negative, we infer that

$$\ln k + \int \left(\ln \frac{d\nu}{d\mu} \right) d\nu < \infty;$$

hence ν obeys the requirements of (7).

(3) With the same notation as in step 2, it follows from (9) that $H(Q,\tilde{P})$ will attain a minimum if and only if

$$\int \left(\ln \frac{d\nu}{d\mu/k} \right) d\nu$$

attains a minimum *and* $Q^z_x = P^z_x$ for ν almost all (x,z) [since only in this case the second summand in (9) attains its minimum, namely zero]. Now assume that (7) holds. Then according to Föllmer[4] (Sec. II.1.3) there exists, among all probability measures ν on $\mathbf{R}^d \times \mathbf{R}^d$ with marginals ν_0, ν_T, a unique probability measure ν^* which minimizes

$$\int \left(\ln \frac{d\nu}{d\mu/k} \right) d\nu,$$

and it is of the form

$$\nu^*(dx,dz) = f(x)g(z)(1/k)\mu(dx,dz).$$

Thus it follows that among all probability measures Q on Ω with marginals $Q[X_0 \in \cdot\,] = \nu_0$, $Q[X_T \in \cdot\,] = \nu_T$ there is a unique one which minimizes $H(Q,\tilde{P})$, and it is of the form

$$\begin{aligned} Q^* &= \int P^z_x \nu^*(dx,dz) \\ &= \int P^z_x f(x)g(z) \frac{1}{k} \sigma(dx) p(0,x;T,z) dz. \end{aligned}$$

Hence, by Proposition 1, Q^* is a Schrödinger bridge specified by p, ν_0, and ν_T. ■

IV. THE FEYNMAN–KAC CASE: SCHRÖDINGER BRIDGES AND LARGE DEVIATIONS

In an important class of examples, $\tilde{P}$ and hence also the Schrödinger bridge occurring in Proposition 2 admit a natural probabilistic interpretation.

Let $((X_s)_{0<s<T}, P_X)$ be the canonical model of an $\mathbf{R}^d$ valued Markov process with continuous paths, generator G_s

and strictly positive transition densities. Let $c = c(s,x)$ be a given bounded measurable scalar field, put

$$P := \exp\left\{\int_0^T c(s,X_s)ds\right\}\cdot P_X \tag{10}$$

and write $p = p(s,x;t,y)$ for the transition densities of P which remain to be strictly positive but do not obey (2) unless $c = 0$. Using the notation of Secs. II and III we have

$$P = \int P_x^z \sigma(dx)p(0,x;T,z)dz,$$

where σ denotes the distribution of X_0 under P_X. Note that (6) is valid due to boundedness of c.

By the Feynman–Kac formula the semigroup belonging to p has generator $G_s + c(s,\cdot)I$, and under suitable smoothness assumptions on G_s and $c(s,x)$, p is the fundamental solution of

$$\left(\frac{\partial}{\partial s} + G_s + c\right)p = 0 \tag{11}$$

(cf. the remark at the beginning of the Introduction); this, however, will not be needed to derive Theorem 2 below.

Let M be an arbitrary fixed upper bound of c, and let W be the process obtained by killing (X,P_X) with rate $M - c(s,X_s)$ between times 0 and T. We recall that $W = (W_s)_{0\leqslant s\leqslant\zeta}$, where ζ is the time until which W survives, is constructed on the probability space $(\Omega\times\mathbf{R}_+,\overline{P})$, where $\overline{P} := P_X\times\pi$ and π is a unit parameter exponential distribution, by putting

$$\zeta((X,t)) := \inf\left\{r>0: \int_0^r (M - c(s,X_s))ds = t\right\}\wedge T;$$

$$W_s := X_s, \quad 0\leqslant s\leqslant\zeta((X,t)).$$

The probability measure $\widetilde{P} = [1/P(\Omega)]P$ is now characterized as follows.

Proposition 3: $\widetilde{P}$ is the distribution of W conditioned that it survives up to time T. More precisely, for any measurable subset B of Ω there holds $\widetilde{P}[B] = \overline{P}[X\in B\,|\,\zeta = T]$.

Proof: For any Borel set B of trajectories we have, using (10)

$$\overline{P}[X\in B\,|\,\zeta = T] = \int P_W(dX)1_B(X)\exp\left\{-MT + \int_0^T c(s,X_s)ds\right\}\left(\int P_W(dX)\exp\left\{-MT + \int_0^T c(s,X_s)ds\right\}\right)^{-1}$$

$$= \int P_W(dX)1_B(X)\exp\left\{\int_0^T c(s,X_s)ds\right\}\left(\int P_W(dX)\exp\left\{\int_0^T c(s,X_s)ds\right\}\right)^{-1} = \frac{P(B)}{P(\Omega)} = \widetilde{P}(B). \quad \blacksquare$$

We will call $\widetilde{P}$ the *distribution of surviving trajectories*. For the rest of the paper, we put $\mu(dx,dz) := \sigma(dx)p(0,x;T,z)dz$, and let ν_0,ν_T be two probability measures on $\mathbf{R}^d$ which obey (7). Proposition 2 now translates immediately into the following.

Theorem 1: Among all probability measures Q on Ω with marginals $Q[X_0\in\cdot] = \nu_0$, $Q[X_T\in\cdot] = \nu_T$, there exists a unique Q^* that minimizes the relative entropy with respect to the distribution $\widetilde{P}$ of surviving trajectories. Moreover, Q^* is a Schrödinger bridge specified by p, ν_0, and ν_T.

In order to obtain a statement on empirical distributions, we have to relax the side conditions on the "exact knowledge" of initial and final distributions.

Proposition 4: For any fixed $\epsilon>0$, there exists a unique solution Q^ϵ of the minimization problem $H(Q,\widetilde{P}) =$ minimum over the set A^ϵ of those probability measures on Ω whose marginals $Q[X_0\in\cdot]$ and $Q[X_T\in\cdot]$ have a Prohorov distance less than or equal to ϵ from ν_0 and ν_T, respectively.

Moreover, Q^ϵ is a Schrödinger bridge specified by p and its marginals $Q^\epsilon[X_0\in\cdot]$, $Q^\epsilon[X_T\in\cdot]$.

Proof: (1) We put

$$H(A^\epsilon,\widetilde{P}) := \inf_{Q\in A^\epsilon} H(Q,\widetilde{P}).$$

Since A^ϵ is convex and $H(A^\epsilon,\widetilde{P})\leqslant H(Q^*,\widetilde{P}) < \infty$, (where Q^* is as in Theorem 1), there exists a uniquely determined probability measure Q^ϵ on Ω with the property that every sequence (P_n) in A^ϵ with $H(P_n,\widetilde{P})\to H(A^\epsilon,\widetilde{P})$ converges toward Q^ϵ in variation (cf. Csiszár,[14] p. 769; there, Q^ϵ is called the generalized I projection of $\widetilde{P}$ on A^ϵ). A fortiori, any such sequence (P_n) converges weakly toward Q^ϵ, and since A^ϵ is weakly closed, we infer that $Q^\epsilon\in A^\epsilon$.

(2) Combining formulas (1.5) and (1.6) of Csiszár,[14] one obtains that $H(Q^\epsilon,\widetilde{P}) = H(A^\epsilon,\widetilde{P})$. On the other hand, any $Q\in A^\epsilon$ with the property $H(Q,\widetilde{P}) = H(A^\epsilon,\widetilde{P})$ necessarily coincides with Q^ϵ due to uniqueness of the generalized I projection.

(3) Denoting the marginals $Q^\epsilon[X_0\in\cdot]$ and $Q^\epsilon[X_T\in\cdot]$ by ν_0^ϵ and ν_T^ϵ, respectively, we consider now the minimization problem $H(Q,\widetilde{P}) =$ minimum over the probability measures Q on Ω with marginals

$$Q[X_0\in\cdot] = \nu_0^\epsilon, \quad Q[X_T\in\cdot] = \nu_T^\epsilon.$$

We know from Proposition 2 that the solution $(Q^\epsilon)^*$ of this problem exists and is a Schrödinger bridge specified by p, ν_0^ϵ and ν_T^ϵ. Since $H((Q^\epsilon)^*,\widetilde{P})\leqslant H(Q^\epsilon,\widetilde{P})$, we infer from step 2 that $(Q^\epsilon)^*$ and Q^ϵ are equal. $\blacksquare$

Given a sequence $X^1,X^2,\ldots$ of i.i.d. random trajectories, each with distribution $\widetilde{P}$, a set Π of probability measures on Ω said to have the *Sanov property* with respect to $\widetilde{P}$ if

$$\lim_{n\to\infty}\frac{1}{n}\ln\text{Prob}\left[\frac{1}{n}\sum_{i=1}^n \delta_{X^i}\in\Pi\right] = -\inf_{Q\in\Pi} H(Q,\widetilde{P}).$$

By Sanov's theorem (see Deuschel and Stroock,[15] p. 70), a sufficient condition for Π to have the Sanov property is

$$\inf_{Q\in\text{int}(\Pi)} H(Q,\widetilde{P}) = \inf_{Q\in\text{cl}(\Pi)} H(Q,\widetilde{P}), \tag{12}$$

where $\text{int}(\Pi)$ and $\text{cl}(\Pi)$ denote the interior and the closure of Π with respect to the weak topology.

Proposition 5: The set A^ϵ defined in Proposition 4 has the Sanov property with respect to $\widetilde{P}$ except possibly for countably many $\epsilon>0$.

Proof: The functions $f(\epsilon) := \inf_{Q \in \text{int}(A^\epsilon)} H(Q,\tilde{P})$ and $g(\epsilon) := \inf_{Q \in \text{cl}(A^\epsilon)} H(Q,\tilde{P})$ both are nonincreasing and hence are continuous except possibly for countably many ϵ. Now let ϵ be a continuity point of f. Since $\text{cl}(A^\epsilon)$ is a subset of $\text{int}(A^\delta)$ for all $\epsilon < \delta$, then $f(\delta) \leqslant g(\epsilon)$ for all $\epsilon < \delta$, and thus also $f(\epsilon) \leqslant g(\epsilon)$. The inequality $f(\epsilon) \geqslant g(\epsilon)$ is obvious. Hence $\Pi := A^\epsilon$ obeys (12), and therefore has the Sanov property with respect to $\tilde{P}$. ■

The above results together with Theorem 1 of Csiszár[14] (and the remarks following that theorem) imply immediately the following result.

Theorem 2: Consider N i.i.d. particles in $\mathbf{R}^d$, each with initial distribution σ, moving according to G_s and being killed independently with rate $M - c(s,x)$, where the constant M is some upper bound of c. Then the "surviving trajectories" $X^1,\ldots,X^n$ are, for $N \to \infty$, asymptotically quasi-independent under the condition

$$\rho\left(\frac{1}{n}\sum_{i=1}^{n}\delta_{X_0^i},\nu_0\right) \leqslant \epsilon, \quad \rho\left(\frac{1}{n}\sum_{i=1}^{n}\delta_{X_T^i},\nu_T\right) \leqslant \epsilon,$$

and their limiting distribution (in the sense of Csiszár[14]) is a Schrödinger bridge specified by p and some ν_0^ϵ and ν_T^ϵ such that $\rho(\nu_0,\nu_0^\epsilon) \leqslant \epsilon$ and $\rho(\nu_T,\nu_T^\epsilon) \leqslant \epsilon$ (where ρ denotes the Prohorov distance, and where $\epsilon > 0$ is chosen such that the set A^ϵ defined in Proposition 4 has the Sanov property with respect to $\tilde{P}$; cf. Proposition 5. For the notion of asymptotic quasi-independence and limiting distribution, we refer to Csiszár,[14] Definition 2.1).

We conclude by formulating a corollary to Theorem 2 in a more qualitative way.

Let p be a fundamental solution of (11), let σ be some probability distribution on $\mathbf{R}^d$, put $\mu(dx, dz) := \sigma(dx)p(0,x;T,z)dz$, and let ν_0, ν_T be given probability distributions on $\mathbf{R}^d$ obeying (7). Consider N i.i.d. particles, each with initial distribution σ, moving according to G_s and being killed independently with rate $M - c(s,x)$, where M is some fixed upper bound of c. Then, for large N, the conditional distribution of the empirical distribution of surviving trajectories, given that the initial and final empirical distributions of surviving trajectories are close to ν_0 and ν_T, respectively, is approximately a Schrödinger bridge specified by p and initial and final marginals which are close to ν_0 and ν_T, respectively.

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Solution of the multivariate Fokker–Planck equation by using a maximum path entropy principle

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This paper proposes an approach via the maximum entropy principle in order to determine the nonstationary solutions of the Fokker–Planck equation with time varying coefficients. The constraints are not the state moments (as usual) but their dynamic equations. The maximum entropy principle herein utilized is a slight extension of Jaynes' principle, which involves the "path entropy" of the stochastic process.

I. INTRODUCTION

The Fokker–Planck equation (FP equation in the following) is a basic tool of theoretical physics, and in many problems such as, for instance, the analysis of the effects of fluctuations close to the transition point, it is more suitable than the Langevin or Itô equation. It is also powerful in the study of stochastic porcesses, and for all these reasons, it is of paramount interest to have efficient methods for obtaining the explicit expression of its solution.

Consider the one-dimensional FP equation

$$\partial_t p(x,t) = -\partial_x [f(x,t)\, p(x,t)] + \tfrac{1}{2}\partial_{xx}[\, g(x,t)\, p(x,t)], \tag{1}$$

where ∂_t (resp. ∂_x) holds for the partial derivative w.r.t. t (resp. x) and ∂_{xx} represents the second partial derivative w.r.t. x; then loosely speaking, there are two main useful techniques that are utilized to find its solutions.

The first one (see, for instance, Risken)[1] considers the special case when $f(x)$ and $g(x)$ are independent of time, and it consists of using eigenfunction expansions. In short, it works as follows: First, by making a suitable change of variable $x' = y(x)$, one transforms Eq. (1) into

$$\partial_t \tilde{p}(y,t) = -\partial_y(\tilde{f}(y)\, \tilde{p}(y,t)) + \tfrac{1}{2}\partial_{yy}\tilde{p}(y,t) \tag{2}$$

and then one looks for nonstationary solutions of (2) in the form

$$\tilde{p}(y,t) = \tilde{p}(y)\exp\{-\lambda t\}, \tag{3}$$

where $\tilde{p}(y)$ and λ are the eigenfunctions and eigenvalues of the FP operator $(-\partial_y \tilde{f} + \tfrac{1}{2}\partial_{yy})$, with appropriate boundary conditions.

The second technique (see, for instance, Kree and Soize)[2] refers to the general case when $f(x,t)$ and $g(x,t)$ depend explicitly upon time. Shortly, one first considers the function $q(x,t)$ defined as

$$q(x,t) := p(x,t)[\phi(x)]^{-1}, \tag{4}$$

$$\phi(x) := (2\pi)^{-1/2}\exp\{-x^2/2\}, \tag{5}$$

and one expands $q(x,t)$ in the form

$$q(x,t) = \sum_{j=0}^{j=\infty} q_j(t)\frac{H_j(x)}{\sqrt{j!}}, \tag{6}$$

where $H_j(x), j = 0,1,2,...$ denotes the Hermite's polynomials [i.e., defined by the equation $H_j(x)g(x) = (-1)^j(d/dx)^j\cdot\phi(x)$]. Second, we substitute (6) into (1), we integrate over R w.r.t. x, and we so obtain an infinite set of first-order linear differential equations to calculate the $q_j(t)$'s.

The troublesome point with this approach is its convergence. Numerical experiments have shown that, as expected, the convergence is as much better as $p(x,t)$ is close to the normal law, but when it is not the case, this convergence becomes questionable.

So, as an alternative, we shall herein suggest a new approach for solving the FP equation, which is mainly based upon the use of Jaynes[3] maximum entropy principle. One of the main advantages of this technique if that it provides the solution in a compact form which is physically more meaningful than the expression by means of series expansions and eigenfunctions, because it is defined directly in terms of the elements of the FP equations.

II. THEORETICAL PRELIMINARIES

A. A characterization of the Fokker–Planck equation

1. Preliminary notations

Let $x(t) \in R^n$, $x^T := (x_1, x_2, ..., x_n)$ denote a stochastic process with the probability density $p(x,t)$, and the increment $z := x(t+\tau) - x(t)$. Define the conditional probability density $q(z,\tau/x,t)$ of z at $t+\tau$ given the state x at t; define the multiindex $\mathbf{k} := (k_1, k_2, ..., k_n)$, $k_i \geqslant 0$ for every i, define

$$\omega^{\mathbf{k}}(x) := x_1^{k_1}x_2^{k_2}\cdots x_n^{k_n} \tag{7}$$

and the moments

$$m_{\mathbf{k}}(t) := \langle \omega^{\mathbf{k}}(x)\rangle. \tag{8}$$

The conditional expectation of $\omega^{\mathbf{k}}(z)$ given x at t will be denoted by $\langle \omega^{\mathbf{k}}(z)/x,t\rangle$ and furthermore the expression $|\mathbf{k}| \geqslant K$ will be shorthand for $k_1 + k_2 + \cdots + k_n \geqslant K$. We can now state the following results.

Proposition 2.1: Consider the continuous stochastic process above, and assume that it is Markovian and satisfies the following conditions:

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$$\langle z_i/x,t\rangle = \tau f_i(x,t); \quad i=1,2,...,n, \tag{9}$$

$$\langle z_i z_j/x,t\rangle = \tau g_{ij}(x,t); \quad i,j=1,2,...,n, \tag{10}$$

$$\langle \omega^k(z)/x,t\rangle = o(\tau^2); \quad |\mathbf{k}|\geqslant 3. \tag{11}$$

Then the moments $m_{\mathbf{k}}$'s are given by the following dynamical equations:

$$\dot{m}_i(t) = \langle f_i(x,t)\rangle, \quad i=(\delta_{1i},\delta_{2i},...,\delta_{ni}), \quad |i|=1, \tag{12}$$

$$\dot{m}_{\mathbf{k}}(t) = \left\langle \sum_{i=1}^{n} f_i \partial_i \omega^{\mathbf{k}}(x) + \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} g_{ij}\partial_{ij}\omega^{\mathbf{k}}(x)\right\rangle$$

$$=: \langle P_{\mathbf{k}}(x,t)\rangle, \quad \mathbf{k}\geqslant 2, \tag{13}$$

with the notations $\partial_i := \partial/\partial x_i$ and $\partial_{ij} := \partial^2/\partial x_i\,\partial x_j$ and where δ_{ij} is the Kronecker delta. ■

Proposition 2.2: Assume that the following conditions are satisfied

(A1) Conditions of proposition (2.1);

(A2) $f_i(x,t)$ and $\partial_j f_i(x,t)$ are continuous and bounded for every pair (i,j) and every $(x,t)\in R^{n+1}$;

(A3) $g_{ij}(x,t)$, $\partial_k g_{ij}(x,t)$, and $\partial_{ks} g_{ij}(x,t)$ are continuous and bounded for every quartet (i,j,k,s) and every $(x,t)\in R^{n+1}$.

Then the moment equations (12) and (13) yield the FP equation

$$\partial_t p = -\sum_{i=1}^{n}\partial_i(f_i p) + \tfrac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} + \partial_{ij}(g_{ij}p) \tag{14}$$

as a consequence, and conversely, the FP equation provides these moment equations. ■

Proposition 2.3: Assume that the following conditions are satisfied

(B1) Conditions of proposition (2.1);

(B2) for every i, $f_i(x,t)$ is a polynomial in the form

$$f_i(x,t) = \sum_{|\mathbf{k}|=0}^{K_i} f_{i\mathbf{k}}(t)\omega_{\mathbf{k}}(x), \tag{15}$$

where $f_{i\mathbf{k}}(t)$ is bounded, $|f_{i\mathbf{k}}(t)|\leqslant M < +\infty$, $0\leq t\leq +\infty$;

(B3) for every pair (i,j), $g_{ij}(x,t)$ is a polynomial in the form

$$g_{ij}(x,t) = \sum_{|k|=0}^{K_{ij}} g_{ij\mathbf{k}}(t)\omega_{\mathbf{k}}(x), \tag{16}$$

where the $g_{ij\mathbf{k}}(t)$ are bounded.

Then the moment equations (12) and (13) yield the FP equation as a consequence and conversely, the FP equation provides these moment equations. ■

For the proof, see for instance Ref. 4.

These results show that, under some mathematical assumptions which are not so much restrictive at all, there is a complete equivalence between the FP equation (14) on the one hand, and the moment equations (12) and (13) on the other hand, in such a manner that, in the following, we shall use the latter to solve the former.

III. SOLUTION VIA THE MAXIMUM PATH ENTROPY PRINCIPLE

A. Extension of the maximum entropy principle

Owing to the fact that the constraints (14) and (13) explicitly involve the derivative of the moments, that is to say $\partial_t p(x,t)$, we shall first generalize the maximum entropy principle as follows.

1. Maximum path entropy principle

Assume that all we know about a stochastic process $x(t)$ is a set of constraints on its probability density $p(x,t)$. Then as an estimate of $p(x,t)$, we shall select that $\hat{p}(x,t)$ which satisfies these constraints and maximizes the entropic function

$$\tilde{H}(X;t',t'') := -\int_{t'}^{t''}\int_{R^n} p(x,t)\ln p(x,t)\,dx\,dt \tag{17}$$

$$= \int_{t'}^{t''} H(X,t)\,dt, \tag{18}$$

for any arbitrary interval $[t',t'']$. ■

The meaning of this statement is quite understandable. For a given fixed interval $[t',t'']$, if $H(X,t)$ is maximum for any $t\in[t',t'']$, then $\tilde{H}(X;t',t'')$ is also maximum. But the converse is not necessarily true, and this is the reason why we require that $[t',t'']$ be arbitrary.

Let us also remark that, by using physical and mathematical arguments, we[5] have shown that $\tilde{H}(X;t',t'')/(t''-t')$ can be considered as the informational engropy of the portion of stochastic trajectory generated by $x(t)$ on the interval $[t',t'']$; clearly, it is a *path entropy* $H(X;t',t'')$.

B. General expression of the probability density estimation

1. Preliminaries

(i) In order to solve the FP equation (14), we shall rewrite the moment equations (12) and (13) in the form

$$\int_{R^n}[x_i\partial_t p(x,t) - f_i(x,t)p(x,t)]\,dx = 0, \tag{19}$$

$$\int_{R^n}[\omega^k(x)\partial_t p(x,t) - p_{\mathbf{k}}(x,t)p(x,t)]\,dx = 0,$$

$$2\leqslant|\mathbf{k}|\leqslant K, \tag{20}$$

where K is the order of the approximation, and we shall consider (19) and (20) as being the constraints.

(ii) Next, we are estimating the solution of the partial differential equation (14), and for a given initial $p(x,t_0)$, this solution is completely well defined at the instants t' and t''. As a result, we shall add the supplementary condition that: $p(x,t')$ and $p(x,t'')$ have given fixed values.

With these prerequisites, we shall proceed as follows.

Step 1: By using the Lagrange multipliers $\tilde{\lambda}_0(t)$, $\lambda_i(t)$, and $\mu_{\mathbf{k}}(t)$, we shall maximize the quantity [indeed we have the additional constraint $\int p(x,t)\,dx = 1$!]

$$\int_{R^n}\int_{t'}^{t''}\Big[-p\ln p+\tilde{\lambda}_0 p+\sum_{i=1}^{n}\lambda_i(t)(x_i\partial_t p-f_i p)$$

$$+\sum_{|\mathbf{k}|=2}^{K}\mu_{\mathbf{k}}(t)(\omega^{\mathbf{k}}(x)\partial_t p-P_{\mathbf{k}}p)\Big]dt\,dx=L \tag{21}$$

and the corresponding variational condition of optimizaton is

$$-\int_{R^n}\int_{t'}^{t''}\Big[\ln p+1+\tilde{\lambda}_0(t)+\sum_i\lambda_i(t)f_i+\sum_{\mathbf{k}}\mu_{\mathbf{k}}(t)P_{\mathbf{k}}\Big]$$

$$\times\delta p(x,t)dt\,dx+\int_{R^n}\int_{t'}^{t''}\Big[\sum_i\lambda_i(t)x_i$$

$$+\sum_{\mathbf{k}}\mu_{\mathbf{k}}(t)\omega^{\mathbf{k}}(x)\Big]\delta(\partial_t p(x,t))dt\,dx=0. \tag{22}$$

Step 2: In order to manipulate the variation $\delta(\partial_t p(x,t))$, we shall write, for instance

$$\int_{R^n}\int_{t'}^{t''}\mu_{\mathbf{k}}(t)\omega^{\mathbf{k}}(x)\delta(\partial_t p(x,t))dt\,dx$$

$$=\int_{R^n}\omega^{\mathbf{k}}(x)\{[\mu_{\mathbf{k}}(t)\delta p(x,t)]_{t'}^{t''}$$

$$-\int_{t'}^{t''}\dot{\mu}_{\mathbf{k}}(t)\delta p(x,t)\}dx\,dt$$

$$=-\int_{R^n}\int_{t'}^{t''}\dot{\mu}_{\mathbf{k}}(t)\omega^{\mathbf{k}}(x)\delta p(x,t)dx\,dt. \tag{23}$$

Step 3: Substituting this result into (22), we obtain the general form of the estimate $\hat{p}_K(x,t)$ which is

$$\hat{p}_K(x,t)=\exp\Big\{-\Big[\lambda_0(t)+\sum_{i=1}^{n}\lambda_i(t)f_i(x,t)$$

$$+\sum_{|\mathbf{k}|=2}^{K}\mu_{\mathbf{k}}(t)P_{\mathbf{k}}(x,t)$$

$$+\sum_{i=1}^{n}\dot{\lambda}_i(t)x_i+\sum_{|\mathbf{k}|=2}^{K}\dot{\mu}_{\mathbf{k}}(t)\omega^{\mathbf{k}}(x)\Big]\Big\}, \tag{24}$$

where $\lambda_0(t)$ holds for

$$\lambda_0(t):=1+\tilde{\lambda}_0(t). \tag{25}$$

C. Determination of the Lagrange multipliers

Step 1: In order to determine the explicit expressions of the vectors

$$\lambda^T(t):=(\lambda_0(t),\lambda_1(t),...,\lambda_n(t))$$

and

$$\mu^T(t):=(\mu_{k_1}(t),\mu_{k_2}(t),...)$$

we shall substitute (24) into the constraints (19) and (20) to obtain a nonlinear vector differential equation in the form

$$A(t,\lambda,\mu)\ddot{\lambda}+B(t,\lambda,\mu)\dot{\lambda}+C(t,\lambda,\mu)\lambda+D(t,\lambda,\mu)\ddot{\mu}$$

$$+E(t,\lambda,\mu)\dot{\mu}+F(t,\lambda,\mu)\mu=b(t,\lambda,\mu), \tag{26}$$

where the matrices A,B,C,D,E,F, and the vector b are defined in terms of the expected values of functions which depend upon both x and t. For instance one has

$$b^T(t,\lambda,\mu):=(...,\langle f_i(x,t)\rangle,...,\langle P_{\mathbf{k}}(x,t)\rangle,...).$$

Step 2: The determination of the solution of (26) is essentially a numerical computation problem, and for instance, one can use the iterative procedure defined by the equation

$$A(t,\lambda_n,\mu_n)\ddot{\lambda}_{n+1}+B(t,\lambda_n,\mu_n)\dot{\lambda}_{n+1}$$

$$+C(t,\lambda_n,\mu_n)\lambda_{n+1}+D(t,\lambda_n,\mu_n)\ddot{\mu}_{n+1}$$

$$+E(t,\lambda_n,\mu_n)\dot{\mu}_{n+1}+F(t,\lambda_n,\mu_n)\mu_{n+1}=b(t,\lambda_n,\mu_n), \tag{27}$$

Step 3. Initial conditions for $\lambda(t)$ and $\mu(t)$: In order to determine these parameters, we shall proceed as follows.

(i) Let us refer to the initial condition $p_0(x):=p(x,t_0)$ and let us assume that one has exactly

$$p_0(x)=\exp\Big\{-\sum_{i=0}^{n}\alpha_i x_i-\sum_{|\mathbf{k}|=2}^{K}\beta_{\mathbf{k}}\omega^{\mathbf{k}}(x)\Big\}, \tag{28}$$

then comparing with (24) directly yields

$$\lambda_0(0)=\alpha_0, \tag{29}$$

$$\lambda_i(0)=\mu_{\mathbf{k}}(0)=0,\quad i\geqslant 1,\quad |\mathbf{k}|\geqslant 2, \tag{30}$$

and

$$\dot{\lambda}_i(0)=\alpha_i,\quad i=1,2,...,n, \tag{31}$$

$$\dot{\mu}_k(0)=\beta_k,\quad 2\leqslant|k|\leqslant K. \tag{32}$$

(ii) Assume now that $p_0(x)$ is not given in the special form (28), then by using a Galerking approximation, for instance, we shall determine α_i and β_k so as to minimize the criterion

$$\min_{\alpha_i,\beta_k}\int_{R^n}\Big[\ln p_0(x)-\Big(\sum_i\alpha_i x_i+\sum_{\mathbf{k}}\beta_{\mathbf{k}}\omega^{\mathbf{k}}(x)\Big)\Big]^2 p_0(x)dx, \tag{33}$$

and we shall use the conditions (29) to (32). ■

Remark of practical interest: In order to initiate the iterative procedure (27), we shall need initial estimates for $\langle f_i(x,t)\rangle$, $\langle P_{\mathbf{k}}(x,t)\rangle$, and the like. To this end, one can select $p_0(x)$, and one will have, for instance

$$\langle f_i(x,t)\rangle_0=\int_{R^n}f_i(x,t)p_0(x)dx.$$

Another alternative is to make the approximation

$$f_i(x,t)\cong x^T\tilde{\mathbf{f}}_i(t),$$

$$g_{ij}(x,t)\cong\tilde{g}_{ij}(t),$$

and to take the normal distribution so defined by the corresponding FP equation

$$\partial_t p=-\sum_i\partial_i(x^T\tilde{f}_i(t)p)+\tfrac{1}{2}\sum_{ij}\tilde{g}_{ij}(t)\partial_{ij}p.$$

For instance, if zero is an equilibrium position for the system in the absence of random inputs, one then has $f_i(0,t)=0$, and one can select

$$f_i(x,t)\cong x^T\partial_x f_i(0,t).$$

Regarding $\tilde{g}_{ij}(t)$, a possible choice is

$$\tilde{g}_{ij}(t):=\int_{R^n}g_{ij}(x,t)p_x(x)dx.$$

Illustrative example: In order to illustrate the procedure, we shall outline the well-known special case defined by the one-dimensional FP equation

$$\partial_t p = -\partial_x(xf(t)p) + \tfrac{1}{2}\partial_{xx}(g(t)p) \tag{34}$$

with the initial condition

$$p(x,0) = \exp\{-\tfrac{1}{2}\ln(2\pi\sigma^2) - (x-x_0)^2/2\sigma^2\}. \tag{35}$$

We bear in mind that the solution of (34) is

$$p(x,t) = [2\pi v(t)]^{-1/2}\exp\{-(x-m_1(t))^2/2v(t)\}, \tag{36}$$

with

$$v(t) := m_2(t) - m_1^2(t),$$
$$\dot{m}_1(t) = f(t)m_1(t), \quad m_1(0) = x_0,$$
$$\dot{m}_2(t) = 2f(t)m_2(t) + g(t), \quad m_2(0) = \sigma^2 + x_0^2.$$

Let us seek the solution of (34) by applying the method above, and let us consider the approximation of the second moment.

(i) One has

$$f(x,t) = xf(t),$$
$$g(x,t) = g(t),$$
$$P_k(x,t) = kf(t)x^k + \tfrac{1}{2}k(k-1)g(t)x^{k-2},$$

and Eq. (24) yields

$$\hat{p}_2(x,t) = \exp\{-[\lambda_0(t) + \mu_2(t)g(t)] - x[\lambda_1(t)f(t) + \dot{\lambda}_1(t)] - x^2[2\mu_2(t)f(t) + \dot{\mu}_2]\} \tag{37}$$

$$= \exp\{-\alpha(t) - x\beta(t) - x^2\gamma(t)\}, \tag{38}$$

where the definition of $\alpha(t)$, $\beta(t)$, and $\gamma(t)$ is obvious.

(ii) We now substitute (38) into the condition

$$\int \hat{p}_2(x,t)dx = 1, \tag{39}$$

and the conditions (19) and (20), to yield

$$\dot{\alpha} + \dot{\beta}\langle x\rangle + \dot{\gamma}\langle x^2\rangle = 0, \tag{40}$$
$$\dot{\alpha}\langle x\rangle + \dot{\beta}\langle x^2\rangle + \dot{\gamma}\langle x^3\rangle = -f(t)\langle x\rangle, \tag{41}$$
$$\dot{\alpha}\langle x^2\rangle + \dot{\beta}\langle x^3\rangle + \dot{\gamma}\langle x^4\rangle = -2f(t)\langle x^2\rangle - g(t), \tag{42}$$

where (40) is obtained by deriving (39) w.r.t. time.

(iii) The initial conditions on $\lambda_i(t)$ and $\mu_2(t)$ are [see Eqs. (29) to (32)]

$$\lambda_0(0) = -\tfrac{1}{2}\ln(2\pi\sigma^2) - (x_0^2/2\sigma^2), \tag{43}$$
$$\lambda_1(0) = 0, \quad \dot{\lambda}_1(0) = x_0/\sigma^2, \tag{44}$$
$$\mu_2(0) = 0, \quad \dot{\mu}_2(0) = -(1/2\sigma^2). \tag{45}$$

(iv) In order to calculate α,β,γ; we need to determine estimates of $\langle x^i\rangle$, $i = 1,...,4$ and to this end we shall take $p(x,t) = p(x,0)$, therefore

$$\langle x\rangle_0 = x_0, \tag{46}$$
$$\langle x^2\rangle_0 = x_0^2 + \sigma^2, \tag{47}$$
$$\langle x^3\rangle_0 = x_0^3 + 3\sigma^2 x_0, \tag{48}$$
$$\langle x^4\rangle_0 = x_0^4 + 6x_0^2\sigma^2 + 3\sigma^4. \tag{49}$$

(v) Substituting (46)–(49) into (40)–(42) yields $(\alpha,\beta,\gamma)_1$ therefore $(\lambda_0(t),\lambda_1(t),\mu_2(t))_1$.

(vi) We now substitute $(\lambda_0(t),\lambda_1(t),\mu_2(t))_1$ into the expression (37) of $\hat{p}_2(x,t)$ and we can then calculate $(\langle x\rangle,\langle x^2\rangle,\langle x^3\rangle,\langle x^4\rangle)_1$ therefore $(\alpha,\beta,\gamma)_2$ and thence $(\lambda_0(t),\lambda_1(t),\mu_2(t))_2$.

And so on.

IV. CONCLUDING REMARKS

In the present paper, we have proposed a new method for determining the solution of the Fokker–Planck equation by directly referring to the dynamical equations of the state moments, considered as constraints in the application of the maximum entropy principle.

The idea of using the moments to estimate the solution of the FP equation can be found in the literature, and Risken[1] has given some methods, but they deal mainly with stationary solutions on the one hand, and transition moments $f(x,t)$ and $g(x,t)$ in polynomial forms w.r.t. x, on the other hand. Recently Haken[6] applied the maximum entropy principle to nonequilibrium phase transitions, but again in the special polynomial case (the laser equation), and by using a perturbation scheme around the stationary solution.

In contrast, the novelty of our approach is the utilization of the "path entropy" that provides the sought solution without referring to the values of the moments themselves. In order to obtain the Lagrange multipliers, we have to solve a set of implicit nonlinear differential equations, but approximate solutions can be easily derived. In addition, we have obtained the general form of the solution (even in the absence of the explicit determination of the Lagrange multipliers) and this feature may be of interest in theoretical studies. On a rigorous standpoint, strictly speaking, we need all the constraints to correctly calculate $p(x,t)$, but numerical experiments have shown that, very often, the first five or six conditions are largely sufficient to achieve a good accuracy.

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Symmetries in predictive relativistic mechanics

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Symmetries of a two-body relativistic harmonic oscillator and a two-body relativistic Coulomb system are considered. It is shown that, in the harmonic case, the Lie algebra of first integrals includes Poincaré algebra and u(3). In the Coulomb case, the Lie algebra of first integrals includes Poincaré algebra and one of the algebras so(1, 3), so(4), or the algebra corresponding to the group of rigid motions in $\mathbb{R}^3$. In both cases, the algebra generated by internal symmetry together with the complete space-time symmetry is infinite dimensional.

I. INTRODUCTION, NOTATIONS, BASIC DEFINITIONS

During the last 20 years, the relativistic theory of directly interacting particles has been intensely developed.[1] In this approach, the field that carries interaction is supposed to be eliminated, and one ends up with an effective action-at-a-distance theory, relevant for a lot of situations in which the creation of particles is not significant whereas other relativistic effects must be taken into account. A great advantage of this approach is the ability to deal with a finite number of degrees of freedom, in a manifestly covariant manner. Relativistic predictive mechanics,[2] especially in its *a priori* Hamiltonian version,[3] is a framework for such investigations. Many explicitly solvable models have been considered in this formalism,[4,5] as well as in alternative but mostly equivalent formulations, based on the use of either the singular Lagrangian or constraints Hamiltonian dynamics.[6]

In so far as we know, the Lie algebra generated by the first integrals of these models was never systematically investigated,[7] although it should obviously help to understand the mechanism of dynamical symmetries from a relativistic viewpoint. In this article, we start such a study, considering only *two-body* systems. (Recall that one-particle problems are trivial from the point of view of predictive mechanics, and inadequate for our purpose, since the presence of an external field destroys space-time symmetry.)

Our analysis will be devoted to the simplest cases of two-particle systems, namely the relativistic oscillator and the system which corresponds to a Coulomb potential. The oscillator is of particular physical interest as it provides a classical prototype of the quark model. The other model is the most naive relativistic generalization of a Coulombian's two-body system. *We shall not try* to use it for a realistic description of gravitational or electromagnetic interaction. Most probably, such a description involves this potential *plus extra terms* which cannot be neglected when relativistic velocities occur.[8] So, the naive Coulombian model can be used as a reference to which the results of a realistic description should be compared eventually.

In the scope of the present work, the relativistic Coulomb potential is mainly interesting because it shares with the harmonic oscillator the property of being exactly solvable in closed form. It is therefore natural to start our search for symmetries by a study of these two models. (Their nonrelativistic counterparts are well known to play particular roles.[9]

These models are not only exactly solvable in abstract form (that is, in terms of abstract canonical variables), but also the so-called position equation which in predictive mechanics determines the relationship between the canonical coordinates and the physical coordinates is tractable in both cases. In fact, this equation was exactly solved for the oscillator, and more generally, for any potential which, in the notations below, writes $V(\vec{z}^2)$, this equation can be reduced to an ordinary differential equation of the Sturm–Liouville type.

This Introduction will be completed by a survey of basic definitions used in our formalism. Sections II and III are, respectively, devoted to the oscillator and the relativistic Coulomb system. A general method for solving the position equations corresponding to a potential $V(\vec{z}^2)$ is indicated in the Appendix.

We shall use the following notation. (a) Flat space-time (M_4, g), where g is the metric tensor on M_4 such that $g_{00} = 1, g_{ij} = -\delta_{ij}$; all other components of g are equal to zero. (b) Greek subscripts run from 0 to 3, Latin from 1 to 3. (c) One-particle phase space $T(M_4)$ is identified with the product of M_4 by the space of four-vectors. (d) Two-particle phase space $M \subset T(M_4) \times T(M_4)$. (e) Set of all smooth functions on M: $\mathcal{F}(M)$. (f) Small characters for Lie algebras, capitals for groups, example SO(4), so(4). (g) For each A^μ, B^μ, we will use:

$$A^\mu B_\mu = A \cdot B.$$

(h) Canonical coordinates $q_1^\alpha, p_1^\alpha, q_2^\alpha, p_2^\alpha$. (i) The projectors onto the space orthogonal to the total momentum:

$$\Pi^\alpha{}_\beta = \delta^\alpha{}_\beta - (P^\alpha P_\beta / P^2),$$

where

$$P^\alpha = p_1^\alpha + p_2^\alpha.$$

(j) For each A^μ, we define:

$$\tilde{A}^\mu = \Pi^\mu{}_\nu A^\nu.$$

Let us briefly recall the definition of two-particle sys-

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tems in predictive mechanics. We consider: (1) two-particle phase space M with canonical coordinates $q_1^\alpha, p_1^\alpha, q_2^\alpha, p_2^\alpha$ and standard Poisson bracket, i.e., the two-argument map:

$$\{\cdot\,,\cdot\}: \mathcal{F}(M)\times\mathcal{F}(M)\to\mathcal{F}(M),$$

such that

$$\{f,g\} = -\{g,f\}, \tag{1.1}$$

$$\{f,gh\} = \{f,g\}h + g\{f,h\}, \tag{1.2}$$

$$\{f,\{g,h\}\} + \{h,\{f,g\}\} + \{g,\{h,f\}\} = 0; \tag{1.3}$$

the only nonvanishing Poisson brackets of the coordinates among themselves are

$$\{q_1^\alpha, p_{1_\beta}\} = \{q_2^\alpha, p_{2_\beta}\} = \delta_\beta^\alpha. \tag{1.4}$$

(2) Two Hamiltonians, i.e., two *scalar* functions H_1 and H_2 over M.

In this work, we consider essentially Poincaré invariant interactions. Therefore, H_1 and H_2 are Poincaré invariant, i.e.,

$$\{H_1,P^\alpha\} = 0, \quad \{H_2,P^\alpha\} = 0,$$

$$\{H_1,M^{\alpha\beta}\} = 0, \quad \{H_2,M^{\alpha\beta}\} = 0, \tag{1.5}$$

where

$$P^\alpha = p_1^\alpha + p_2^\alpha, \tag{1.6}$$

$$M^{\alpha\beta} = q_1^\alpha p_1^\beta - q_1^\beta p_1^\alpha + q_2^\alpha p_2^\beta - q_2^\beta p_2^\alpha. \tag{1.7}$$

Moreover, H_1 and H_2 satisfy the predictivity condition:

$$\{H_1,H_2\} = 0. \tag{1.8}$$

(3) Relationship between the positions x_1^α, x_2^α and canonical coordinates is established by solving the position equations:

$$\{H_1,x_2^\alpha\} = \{H_2,x_1^\alpha\} = 0. \tag{1.9}$$

For the reader who is not familiar with the formalism, some remarks are useful.

First, we are dealing with a two-time formalism. The evolution of the system can be written in terms of two independent parameters, each one associated with each particle's proper time. According to this point of view, the time development is generated by two scalar functions H_1, H_2. These functions generate two Hamiltonian vector fields on the symplectic manifold M, which justifies our terminology.

In this scheme, the Hamiltonians are interpreted as proportional to the squared masses, which are automatically constants of the motion. (In contrast, the energy is simply the time component of the linear momentum. We do not use it as a generator.)

In agreement with a famous theorem,[10] the physical variables x_1, x_2 cannot be canonical. Thus the system is not completely defined unless a solution of Eq. (1.9) is chosen. In so far as solvable models are concerned, one usually demands that x_1, x_2 reduce to q_1, q_2 on the 15-dimensional manifold $P\cdot(q_1 - q_2) = 0$. This requirement is interpreted as an equal-time condition in the center-of-mass frame. There are cases where one may alternatively consider an asymptotic condition, namely, that $\tilde{x}_1 - \tilde{x}_2$ coincide with $\tilde{q}_1 - \tilde{q}_2$ at spatial infinity. Naturally, it is essential that the Poincaré symmetry not be destroyed when passing from the physical coordinates to the canonical ones. In other words, it must be possible to define the Poincaré group equivalently by its quadratic invariants as well in terms of q, p as in terms of position and velocities. This condition ensures that P^α and $M_{\mu\nu}$ are not only an arbitrary representation of the *abstract* Poincaré Lie algebra, but are correctly related to space-time symmetry. Solutions based on invariant Cauchy data imposed on the invariant manifold $P\cdot(q_1 - q_2) = 0$ obviously satisfy this condition.

Finally, it is worthwhile to notice that, generally, our phase space M does not cover the whole $T(M_4)\times T(M_4)$. Consider for instance the oscillator. The potential $k(\tilde{q}_1 - \tilde{q}_2)^2$ is singular for null values of P^α. The relevant part of $T(M_4)\times T(M_4)$ is necessarily an open set satisfying $P^2 \neq 0$. For obvious physical reasons, we actually define M by the condition that $P^2 > 0$ and P oriented toward the future. Since P^α is a constant of the motion, this restriction is consistent. Moreover, we shall see that the formula which solves Eq. (1.9) for this model blows up when $P\cdot p_1$ or $P\cdot p_2$ (which fortunately are constants of the motion) vanish. Hence, a further restriction of M, by the conditions $P\cdot p_1 \neq 0$, $P\cdot p_2 \neq 0$.

For any two-body relativistic system formulated as in (1), (2), and (3), a first integral is by definition a function $f\in\mathcal{F}(M)$ such that

$$\{f,H_1\} = \{f,H_2\} = 0. \tag{1.10}$$

From the Jacobi identity (1.3), it follows that such functions form a Lie algebra with respect to the Poisson bracket. This Lie algebra is the principal subject of our paper. Any subalgebra of it is by definition *a dynamical algebra*. It is of particular interest to exhibit finite-dimensional dynamical algebras.

Equations (1.5) and (1.8) together with the definition (1.10) show that, for each two-particle relativistic predictive system the quantities, H_1, H_2, P^α, and $M^{\alpha\beta}$ are first integrals. Since P^α, $M^{\alpha\beta}$ satisfy the commutation relations:

$$\{P^\alpha,P^\beta\} = 0, \tag{1.11a}$$

$$\{M^{\alpha\beta},P^\gamma\} = g^{\alpha\gamma}P^\beta - g^{\beta\gamma}P^\alpha, \tag{1.11b}$$

$$\{M^{\alpha\beta},M^{\gamma\delta}\} = -g^{\beta\gamma}M^{\alpha\delta} + g^{\beta\delta}M^{\alpha\gamma} + g^{\alpha\gamma}M^{\beta\delta} - g^{\alpha\delta}M^{\beta\gamma}, \tag{1.11c}$$

which are the well-known relations for Poincaré algebra, it is clear that symmetries of each predictive two-particle system include Poincaré algebra.

Let us consider two particular predictive relativistic systems, namely,

$$H_1 = \tfrac{1}{2}(\tfrac{1}{2}P + y)^2 + k\tilde{z}^2, \quad H_2 = \tfrac{1}{2}(\tfrac{1}{2}P - y)^2 + k\tilde{z}^2 \tag{1.12}$$

and

$$H_1 = \frac{1}{2}\left(\frac{1}{2}P + y\right)^2 + \frac{\alpha}{\sqrt{-\tilde{z}^2}},$$

$$H_2 = \frac{1}{2}\left(\frac{1}{2}P - y\right)^2 + \frac{\alpha}{\sqrt{-\tilde{z}^2}}, \tag{1.13}$$

where $k > 0$, α are constants, and relative variables are introduced through the notations

$$P^\alpha = p_1^\alpha + p_2^\alpha, \quad Q^\alpha = \tfrac{1}{2}(q_1^\alpha + q_2^\alpha),$$
$$y^\alpha = \tfrac{1}{2}(p_1^\alpha - p_2^\alpha), \quad z^\alpha = q_1^\alpha - q_2^\alpha. \tag{1.14}$$

One can easily check that systems (1.12) and (1.13) satisfy conditions (1.5) and (1.8). They are natural relativistic generalizations of the two-particle nonrelativistic harmonic oscillator[3,4] and the two-particle Kepler system, respectively. They reduce to the system of two noninteracting particles for $k = 0$ and $\alpha = 0$. In both cases, the interaction is carried by a potential, depending only on $\tilde{z}^2$, which is added to the free-particle Hamiltonians.

The position equation (1.9) has been explicitly solved for (1.12).[4] For any potential of the form $V(\tilde{z}^2)$, the general form of its solution is known, up to the determination of two scalar functions which depend on the shape of V.[11] We indicate, in the Appendix, how each one of these functions can be separately calculated. The method applies, in particular, to the Coulomb case.

A further motivation for the study of oscillator and Kepler potential is that their nonrelativistic counterparts are known to play particular roles with respect to dynamical symmetries.[9] And, in fact, we shall see in the following sections that the Lie algebra of first integrals associated with (1.12), resp. (1.13), includes finite-dimensional subalgebras that are the same as in the relativistic analog.

II. THE OSCILLATOR

The system (1.12) describing the two-particle relativistic oscillator was first suggested by one of us (D-V).[3,4] In this model, the relative inertia-momentum tensor

$$N^{\alpha\beta} = (1/\sqrt{2k})\tilde{y}^\alpha\tilde{y}^\beta + \sqrt{2k}\,\tilde{z}^\alpha\tilde{z}^\beta \tag{2.1}$$

is a first integral of the system (1.12). Looking for the Poisson brackets $\{N^{\alpha\beta},N^{\gamma\delta}\}$, we see that it is convenient to introduce the tensor

$$\tilde{M}^{\alpha\beta} = \Pi^\alpha{}_\mu \Pi^\beta{}_\nu M^{\mu\nu}. \tag{2.2}$$

Since P^α and $M^{\alpha\beta}$ are first integrals of the system (1.12), we see that $\Pi^\alpha{}_\mu$ and $\tilde{M}^{\alpha\beta}$ are first integrals, too.

Let us consider the Lie algebra generated by P^α, $M^{\alpha\beta}$, $N^{\alpha\beta}$, and $\tilde{M}^{\alpha\beta}$ and their Poisson brackets. We have

$$\{P^\alpha,P^\beta\} = 0, \tag{2.3a}$$
$$\{M^{\alpha\beta},P^\gamma\} = g^{\alpha\gamma}P^\beta - g^{\beta\gamma}P^\alpha, \tag{2.3b}$$
$$\{M^{\alpha\beta},M^{\gamma\delta}\} = -g^{\beta\gamma}M^{\alpha\delta} + g^{\beta\delta}M^{\alpha\gamma} + g^{\alpha\gamma}M^{\beta\delta} - g^{\alpha\delta}M^{\beta\gamma}, \tag{2.3c}$$
$$\{N^{\alpha\beta},N^{\gamma\delta}\} = \Pi^{\beta\gamma}\tilde{M}^{\alpha\delta} + \Pi^{\beta\delta}\tilde{M}^{\alpha\gamma} + \Pi^{\alpha\gamma}\tilde{M}^{\beta\delta} + \Pi^{\alpha\delta}\tilde{M}^{\beta\gamma}, \tag{2.4a}$$
$$\{\tilde{M}^{\alpha\beta},N^{\gamma\delta}\} = -\Pi^{\beta\gamma}N^{\alpha\delta} - \Pi^{\beta\delta}N^{\alpha\gamma} + \Pi^{\alpha\gamma}N^{\beta\delta} + \Pi^{\alpha\delta}N^{\beta\gamma}, \tag{2.4b}$$
$$\{\tilde{M}^{\alpha\beta},\tilde{M}^{\gamma\delta}\} = -\Pi^{\beta\gamma}\tilde{M}^{\alpha\delta} + \Pi^{\beta\delta}\tilde{M}^{\alpha\gamma} + \Pi^{\alpha\gamma}\tilde{M}^{\beta\delta} - \Pi^{\alpha\delta}\tilde{M}^{\beta\gamma}, \tag{2.4c}$$
$$\{M^{\alpha\beta},\tilde{M}^{\gamma\delta}\} = -g^{\beta\gamma}\tilde{M}^{\alpha\delta} + g^{\beta\delta}\tilde{M}^{\alpha\gamma} + g^{\alpha\gamma}\tilde{M}^{\beta\delta} - g^{\alpha\delta}\tilde{M}^{\beta\gamma}, \tag{2.5a}$$
$$\{M^{\alpha\beta},N^{\gamma\delta}\} = -g^{\beta\gamma}N^{\alpha\delta} - g^{\beta\delta}N^{\alpha\gamma} + g^{\alpha\gamma}N^{\beta\delta} + g^{\alpha\delta}N^{\beta\gamma}, \tag{2.5b}$$
$$\{P^\gamma,\tilde{M}^{\alpha\beta}\} = 0, \tag{2.5c}$$
$$\{P^\gamma,N^{\alpha\beta}\} = 0. \tag{2.5d}$$

The expressions (2.3)–(2.5) show that first integrals (1.6), (1.7), (2.1), (2.2), *do not close* to a Lie algebra. The Lie algebra generated by their successive Poisson brackets is infinitely dimensional. The cause of it is the appearance of projectors $\Pi^{\alpha\beta}$ in the formulas (2.4), which spoils the parallelism with nonrelativistic theory. But we shall show that these projectors can be avoided if, from the first integrals (1.6), (1.7), (2.1), and (2.2), we extract a suitable set of functionally independent (nonlinear) combinations.

To see it, let us notice identities:

$$P^\alpha N_{\alpha\beta} = P^\beta N_{\alpha\beta} = 0, \quad N_{\alpha\beta} = N_{\beta\alpha}, \tag{2.6a}$$
$$P^\alpha \tilde{M}_{\alpha\beta} = P^\beta \tilde{M}_{\alpha\beta} = 0, \quad \tilde{M}_{\alpha\beta} = -\tilde{M}_{\beta\alpha}. \tag{2.6b}$$

They show that $N_{\alpha\beta}$ consists of six and $\tilde{M}_{\alpha\beta}$ of three independent functions.

Let us now consider an arbitrary frame in space-time. Define the matrix $\Lambda^\mu{}_\nu$ such that

$$\Lambda^0{}_\mu = P_\mu/\sqrt{P^2},$$
$$\Lambda^i{}_\mu = \delta^i{}_\mu - P^i\Lambda_\mu, \tag{2.7}$$

where

$$\Lambda^\mu = \begin{cases} 1/\sqrt{P^2}, \\ (P^0/\sqrt{P^2} - 1)(P^k/\mathbf{P}^2) \end{cases},$$
$$\mathbf{P}^2 = -\delta_{ij}P^iP^j.$$

In other words, Λ is a Lorentz matrix that transforms all tensors to the rest frame of the center-of-mass; $\tilde{M}'$ and N' are just M and N transformed to this frame. This matrix has the following properties:

$$\Lambda^\mu{}_\nu\Lambda^\rho{}_\sigma\delta^{\nu\sigma} = g^{\mu\rho}, \tag{2.8a}$$
$$\Lambda^0{}_\rho\Pi^\rho{}_\mu = 0, \tag{2.8b}$$
$$\Lambda^j{}_\rho\Pi^\rho{}_\mu = \Lambda^j{}_\mu, \tag{2.8c}$$
$$\Lambda^j{}_\nu P^\nu = 0, \tag{2.8d}$$
$$\{\Lambda^\mu{}_\nu,\tilde{M}^{\alpha\beta}\} = \{\Lambda^\mu{}_\nu,N^{\alpha\beta}\} = 0. \tag{2.8e}$$

Moreover, $\Lambda^\mu{}_\nu$ is a first integral of the system (1.12), because its matrix elements are functions of P^α only.

Using $\Lambda^\mu{}_\nu$, we shall extract nine independent first integrals from $N_{\alpha\beta}$ and $\tilde{M}^{\alpha\beta}$. In order to do it, we define:

$$N'^{\alpha\beta} = \Lambda^\alpha{}_\mu\Lambda^\beta{}_\nu N^{\mu\nu}, \tag{2.9a}$$
$$\tilde{M}'^{\alpha\beta} = \Lambda^\alpha{}_\mu\Lambda^\beta{}_\nu\tilde{M}^{\mu\nu}. \tag{2.9b}$$

It is obvious that

$$\tilde{M}'^{\alpha\beta} = -\tilde{M}'^{\beta\alpha}, \quad N'^{\alpha\beta} = N'^{\beta\alpha}, \tag{2.10}$$

and Eq. (2.8b) shows that

$$\tilde{M}'^{0\beta} = \tilde{M}'^{\beta 0} = N'^{0\beta} = N'^{\beta 0} = 0. \tag{2.11}$$

The remaining components of $N'^{\alpha\beta}$ and $\tilde{M}'^{\alpha\beta}$ are first integrals of the system (1.2) (they are built as products of first integrals) and satisfy the following relations:

$$\{\tilde{M}'^{ij},\tilde{M}'^{kl}\} = \delta^{jk}\tilde{M}'^{il} - \delta^{jl}\tilde{M}'^{ik} - \delta^{ik}\tilde{M}'^{jl} + \delta^{il}\tilde{M}'^{jk}, \tag{2.12a}$$

$$\{\tilde{M}'^{ij},N'^{kl}\} = \delta^{jk}N'^{il} + \delta^{jl}N'^{ik} - \delta^{ik}N'^{jl} - \delta^{il}N'^{jk}, \tag{2.12b}$$

$$\{N'^{ij},N'^{kl}\} = -\delta^{jk}\tilde{M}'^{il} - \delta^{jl}\tilde{M}'^{ik} - \delta^{ik}\tilde{M}'^{jl} - \delta^{il}\tilde{M}'^{jk}, \tag{2.12c}$$

what can be checked using (2.8), (2.5), and (2.4).

These are the familiar commutation relations for the U(3) Lie algebra.[6] Expressions (2.3) and (2.12) show that the set of first integrals of our system includes a subalgebra (spanned by $\tilde{M}'^{ij}$ and N'^{ij}) isomorphic to the Lie algebra of U(3). Because $\{\Lambda^{\mu}{}_{\nu},M^{\rho\sigma}\}\neq 0$, the brackets $\{M^{\alpha\beta},\tilde{M}'^{ij}\}$ *are not* linear combinations of $P^{\alpha},M^{\mu\nu},\tilde{M}'^{ij},N'^{kl}$, so the vector space spanned by $\tilde{M}'^{ij},N'^{kl}$ and the generators of the Poincaré group *is not* a Lie algebra. In contrast, the algebra generated by $\tilde{M}'^{ij}$ and N'^{kl} can be trivially extended by a direct sum with the algebra of space-time translations.

Notice that the separation of space from time among the components of Λ only depends on the choice of an arbitrary direction in space-time, which corresponds to the rest frame of some inertial observer. For each inertial observer, the above procedure associates a different dynamical algebra isomorphic to the Lie algebra of U(3).

III. THE COULOMB-LIKE SYSTEM

Let us take the most naive generalization of Coulomb interaction, given by the Hamiltonians (1.13). It is easy to see that the predictive relativistic analog of Runge–Lenz vector, namely,

$$R_{\mu} = -\tilde{z}_{\mu}V + \tilde{y}^{\sigma}\tilde{M}_{\sigma\mu}, \tag{3.1}$$

where

$$V = \alpha(-\tilde{z}^2)^{-1/2}$$

is a first integral of the motion generated by H_1, H_2. Indeed, we can notice that only spatial relative variables are involved in R_{μ}. Thus the evolution of R_{μ} is in fact governed by $\{R_{\mu},h\}$ where

$$2h = \tilde{y}^2 + 2V. \tag{3.2}$$

With the help of the useful formulas:

$$\{\tilde{z}_{\alpha},\tilde{y}_{\beta}\} = \Pi_{\alpha\beta},$$

$$\{\tilde{z},h\} = \tilde{y},$$

$$\{\tilde{y}_{\alpha},h\} = -\frac{\partial V}{\partial \tilde{z}^{\alpha}},$$

and setting

$$\rho^2 = -\tilde{z}^2,$$

hence

$$\frac{\partial \rho}{\partial \tilde{z}_{\sigma}} = -\frac{1}{\rho}\tilde{z}_{\sigma},$$

we find

$$\{R_{\mu},h\} = -\tilde{y}_{\mu}\left(V + \rho\frac{dV}{d\rho}\right),$$

which vanishes as a consequence of the "Coulomb" form assumed for $V(\rho)$. A tedious but straightforward calculation, analogous to its nonrelativistic counterpart, provides

$$\{R^{\beta},R^{\delta}\} = -2h\tilde{M}^{\beta\delta}. \tag{3.3}$$

In Eq. (3.3), we notice that h is a constant of the motion which, being manifestly invariant by rotation, has a vanishing bracket with angular momentum. In particular,

$$\{h,\tilde{M}^{\alpha\beta}\} = 0. \tag{3.4}$$

This remark permits us to set Eq. (3.3) in a more convenient form. To do this, we introduce

$$\epsilon = -\operatorname{sign} h,$$

that is to say

$$\epsilon = -1,0,+1,$$

when $h>0$, $h=0$, $h<0$, respectively.

So doing, we split phase space into three invariant pieces $M^{(-)},M^{(0)},M^{(+)}$, which are manifolds of dimensions 16, 15, 16, respectively. Here, $M^{(-)}$ corresponds to the case where $\tilde{y}^2$ and V are of opposite signs (remind that $\tilde{y}^2$ cannot be positive according to the choice of signature). This occurs for $\alpha>0$ (Kepler-like motion, attractive force), on the orbits where $\tilde{z}^2$ remains bounded.

By analogy with the well-known nonrelativistic theory, we define

$$K^{\alpha} = R/\sqrt{2h}, \quad \text{for } \epsilon\neq 0$$

and simply

$$K^{\alpha} = R^{\alpha}, \quad \text{when } \epsilon = 0. \tag{3.5}$$

Now, we compute $\{K^{\alpha},K^{\beta}\}$ with the help of (3.3). Since $\{h,R_{\alpha}\}$ vanishes, we obtain easily

$$\{K^{\alpha},K^{\beta}\} = \epsilon\tilde{M}^{\alpha\beta}. \tag{3.6}$$

Besides, it is straightforward to calculate

$$\{M^{\alpha\beta},R^{\delta}\} = g^{\alpha\delta}R^{\beta} - g^{\beta\delta}R^{\alpha}, \tag{3.7}$$

which yields

$$\{M^{\alpha\beta},K^{\delta}\} = g^{\alpha\delta}K^{\beta} - g^{\beta\delta}K^{\alpha}$$

and, in particular,

$$\{\tilde{M}^{\alpha\beta},K^{\delta}\} = \Pi^{\alpha\delta}K^{\beta} - \Pi^{\beta\delta}K^{\alpha}. \tag{3.8}$$

Consider Eqs. (3.6)–(3.8) together with (2.4c). Similarly, as in the oscillator case, the appearance of the projector $\Pi^{\alpha}{}_{\beta}$ in (3.8) and (2.4c) forbids that the Poisson brackets of $K^{\alpha},\tilde{M}^{\mu\nu}$ close to a Lie algebra. However, using the matrix Λ defined in (2.7), we can eliminate as follows the projectors from (3.8), (2.4c).

In order to do it, let us consider $\tilde{M}'$ as in Eq. (2.9b), and define

$$K'^{\alpha} = \Lambda^{\alpha}{}_{\gamma}K^{\gamma}. \tag{3.9}$$

Because of (2.8), we have

$$K'^0 = \tilde{M}'^{\alpha 0} = \tilde{M}'^{0\alpha} = 0. \tag{3.10}$$

Commutation relations between the remaining components of K'^{α} and $\tilde{M}'^{\alpha\beta}$ are

$$\{K'^i, K'^j\} = \epsilon \tilde{M}'^{ij}, \tag{3.11a}$$

$$\{\tilde{M}'^{ij}, K'^k\} = -\delta^{ik}K'^j + \delta^{jk}K'^i, \tag{3.11b}$$

$$\{\tilde{M}'^{ij}, \tilde{M}'^{kl}\} = \delta^{jk}\tilde{M}'^{il} - \delta^{jl}\tilde{M}'^{ik} - \delta^{ik}\tilde{M}'^{jl} + \delta^{il}\tilde{M}'^{jk}. \tag{3.11c}$$

These relations describe the following Lie algebras:[12] (i) so(4) for $\epsilon < 0$. (ii) For $\epsilon = 0$, we have the Lie algebra $\mathscr{A}$ of the semidirect product of SO(3) and a tridimensional Abelian group (rigid motions in Euclidian space $\mathbb{R}^3$). (iii) so(1, 3) for $\epsilon > 0$.

Expressions (3.11) show that the first integrals of our system include a subalgebra, spanned by $\tilde{M}'^{ij}$ and K'^l, isomorphic to so_4, $\mathscr{A}$, so(1, 3), respectively, for ϵ negative, zero, positive. Since the brackets $\{M^{\alpha\beta}, \tilde{M}'^{ij}\}$ *do not* produce linear combinations of P^{α}, $M^{\mu\nu}$, $\tilde{M}'^{ij}$, N'^{kl}, the vector space spanned by $\tilde{M}'^{ij}$, K'^l, and the generators of the Poincaré group *is not* a Lie algebra. In contrast, the algebra generated by $\tilde{M}'^{ij}$ and K'^l can be trivially extended by direct sum with the algebra of space-time translations.

IV. CONCLUSION AND OUTLOOK

Finally, the Poincaré algebra is combined with the Lie algebra of a symmetry of the relative motion (internal symmetry) through their embedding into a large infinite-dimensional Lie algebra.

The internal symmetry has the same abstract structure as in the corresponding nonrelativistic system. But, by a sort of degeneracy with respect to the case of Galilean mechanics, *the internal symmetry algebra is realized in infinitely many ways*. Indeed, to each inertial observer corresponds a representation of the internal Lie algebra. In so far as we consider simultaneously all these algebras on the same footing, we preserve manifest covariance.

In the present scheme, internal symmetries exactly commute with space time translations, hence with P^2. Thus, if we anticipate quantization, it seems that (in spite of the fact that O'Raifeartaigh's theorem[13] does not deal with infinite-dimensional algebras) an eventual mass splitting of multiplets should be expected *only if* the potential is modified by extra terms.

The possibility to combine space-time and internal symmetries within an infinite-dimensional Lie algebra has been considered already many years ago, but, soon faced the criticism of a tremendous arbitrariness, especially with respect to the interpretation of the infinitely many additional generators that are necessary in order to span this big algebra.[14]

Here, in contrast, the only arbitrariness lies in the construction of the relativistic dynamical system. Once the shape of the potential has been fixed, the structure of the algebra of first integrals is locally independent of the way in which the position equations are solved. But the dynamical interpretation of its generators is possible only after the position equations have been solved (just like is possible the determination of the world lines).

In the two examples treated above, a reasonable solution of the position equations is available in closed form. In such models, we can express each first integral in terms of physical positions and velocities, which permits us to assign a precise dynamical meaning to all the generators of the algebra formed by these first integrals. We hope that these models illustrate the advantage of a true dynamical construction over purely group theoretical approaches.

Further investigation is needed in order to determine if a part of the present analysis can be carried out in the global sense, looking for a symmetry *group* instead of a Lie algebra.

For the moment, a quantum mechanical treatment seems more promising; then the introduction of an external field would be of great interest.

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APPENDIX: SOLUTION TO EQS. (1.9) FOR $V = F(\tilde{z}^2)$

It has been proposed by one of us (Ph.D-V) to look for[4] solution of the form:

$$x_1 = q_1 - (P\cdot p_2/P^2)(\varphi_2 \tilde{z} + \psi_2 \tilde{y}), \tag{A1}$$

$$x_2 = q_2 + (P\cdot p_1/P^2)(\varphi_1 \tilde{z} + \psi_1 \tilde{y}). \tag{A2}$$

Since φ_2, ψ_2 can be obtained from φ_1, ψ_1 by particle exchange, it is enough to look for φ_1, ψ_1. Dropping the particle label, we shall write simply φ, ψ.

Let X be the Hamiltonian vector field generated by H_1, that is

$$XA = \{A, H_1\}, \quad \forall A \in \mathscr{F}(M).$$

Setting

$$\theta = P\cdot z/P\cdot p_1, \tag{A3}$$

we have

$$X\theta = 1. \tag{A4}$$

It was shown in Ref. 4 that the equations in (1.9) which involve φ and ψ then become

$$\varphi = -X\psi, \tag{A5}$$

$$(X^2 + 2F')\psi + 2F'\theta = 0, \tag{A6}$$

with

$$F' = \frac{dF}{d(\tilde{z}^2)}$$

and that

$$X\tilde{z}^2 = -2\eta\sqrt{2\zeta(V-h) - l^2}, \tag{A7}$$

with h defined as in (3.2),

$$l^2 = \tilde{z}^2\tilde{y}^2 - (\tilde{z}\cdot\tilde{y})^2 \tag{A8}$$

and

$$\eta = \text{sign of } \tilde{z}\cdot\tilde{y}.$$

For the Coulomb case, the equations of motion show explicitly that, if we allow $\tilde{z}^2$ to vary, then $\tilde{z}\cdot\tilde{y}$ changes its sign when it vanishes (which occurs at perihelion and aphelion).

Remark: $\tilde{z}^2$ cannot be positive, and l^2 cannot be negative, since $\tilde{z}$ and $\tilde{y}$ are space-like.

Now, let us define χ by

$$\psi = \theta + \chi. \tag{A9}$$

Equation (6) gets simplified as

$$(X^2 + 2F')\chi = 0. \tag{A10}$$

In the oscillator case, F' is a constant, and Eq. (A6) was explicitly solved by demanding that χ depends only on θ (and possibly first integrals of the motion). But, in general, F' depends nontrivially on $\tilde{z}^2$, which makes such requirement inconsistent. In view of this difficulty, let us introduce a new quantity ξ which behaves like θ under action of X:

$$X\xi = 1, \tag{A11}$$

but actually depends on $\tilde{z}^2$. It is easy to see that ξ must be of the form:

$$\xi = \int \frac{d\zeta}{f}, \tag{A12}$$

where $f = X\tilde{z}^2$ is given by (A7), as an explicit function of ζ. In general, χ might depend on 16 independent variables which can be θ, ξ, and 14 independent first integrals of the motion. But we are not concerned with the most general solution of (A6). The one we look for must be as simple as possible and satisfy some reasonable boundary or asymptotic condition. So, let us assume additionally that χ only depends on ξ. (And possibly first integrals of our dynamical system. It is clear that the constants of the motion play the role of ignorable variables.) Now, Eq. (A6) reduces to

$$\left(\frac{d^2}{d\xi^2} + 2F'\right)\chi = 0, \tag{A13}$$

in which F' must be considered as a function of ξ through the change of variable (A12), which implies a dependence on the first integrals h and l^2 through Eq. (A7). Equation (A13) is an ordinary differential equation of the Sturm–Liouville type. The behavior of its solutions depend on the shape of F' as a function of ξ, and can be analyzed by standard methods.

Setting $\rho = \sqrt{\zeta}$, we have in the Coulomb case

$$F' = (\alpha/2)\rho^{-3} \tag{A14}$$

and

$$V\zeta = \alpha\rho,$$

$$f = -2\eta D(\rho),$$

where

$$D = (2\alpha\rho - 2h\sqrt{\rho} - l^2)^{1/2}.$$

So, Eq. (A12) yields

$$\xi = -\tfrac{1}{2}\eta I,$$

where, for instance if $h < 0$:

$$I = -(D/2h) - 2\alpha(-2h)^{-3/2}\log(D - 4h\rho + 2\alpha),$$

which defines implicitly $\rho(\xi)$, to be inserted in (A14).

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On the mixing-enhancing structure of a class of quantum dynamical semigroups

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A sufficient condition for a dissipative evolution to give rise to an ever more chaotic state is obtained and the structure of the corresponding density matrix is studied. As a byproduct, the equation of motion in the Schrödinger picture is, in some cases, explicitly solved.

I. INTRODUCTION

It has been shown recently[1] under which optimal conditions on the generator of a quantum dynamical semigroup does the entropy of a system increase.

This behavior is by itself strongly indicative of irreversibility and progressive loss of information about the system while it is evolving according to a semigroup of contractions.

There exists, however, a deeper analysis of the amount of uncertainty inherent to the state of a quantum system that makes use of the concept of mixing enhancing.[2–4]

This is, in turn, connected with the possibility of partially ordering density matrices by considering their eigenvalues: it is indeed clear that with more states present in a mixture our knowledge of the system is poorer.[5]

On the other hand, an increasing of the smaller eigenvalues together with a decreasing of the bigger ones until they eventually become equal should produce an ever greater lack of information, e.g., in finite systems the most mixed (chaotic) state is the trace $\hat{\mathbf{1}}/N$, N being the dimension.[5]

This is the typical situation when a state (density matrix) $\hat{\rho}$ suffers deleting off-diagonal elements in a given representation as it happens in the usual scheme of a measurement process:

$$\hat{\rho}\to\sum_i P_i\hat{\rho}P_i, \quad P_iP_j=\delta_{ij}P_i, \quad \sum_i P_i=\text{identity};$$

or, when $\hat{\rho}$ undergoes a coarse graining:[5]

$$\hat{\rho}\to\sum_i \frac{\operatorname{Tr} P_i\hat{\rho}}{\operatorname{Tr} P_i}P_i.$$

Since the time-decaying of the off-diagonal elements of $\hat{\rho}$ in the position representation is one of the main features of a model[6] introduced recently to overcome the conceptual difficulties arising in connection with linear superpositions of far away localized macrostates, it seems to be appropriate discussing its properties from the point of view of mixing enhancing.

More generally, it should be noticed that loss of information in the sense sketched above is not a consequence but rather one of the possible reasons for the increasing of entropy.

II. MIXING-ENHANCING PROPERTY OF CERTAIN QUANTUM DYNAMICAL SEMIGROUPS

In order to make more precise the basic ideas outlined in the Introduction, following Refs. 2–4 we will make the following statements.

Definition 2.1: (i) Given two density matrices $\hat{\rho}$ and $\hat{\sigma}$ whose eigenvalues $\{\rho_i\}_{i\in N}$ and $\{\sigma_j\}_{j\in N}$ are arranged in decreasing order, $\hat{\rho}$ is defined to be more mixed than $\hat{\sigma}$ ($\hat{\rho}\vdash\hat{\sigma}$) if

$$\rho(n)\equiv\sum_{i=1}^{n}\rho_i\leqslant\sigma(n)\equiv\sum_{i=1}^{n}\sigma_i, \quad \forall n\in\mathbf{N}.$$

(ii) A map $T[\,\cdot\,]$ from the state space into itself, which transforms density matrices into density matrices, is mixing enhancing if $T[\hat{\rho}]\vdash\hat{\rho}$ for any density matrix $\hat{\rho}$.

Remarks 2.2: (1) The state space we are referring to is usually taken to be the self-adjoint part, $B(\mathscr{H})_1^{\text{s.a.}}$, of the Banach space of the trace-class operators, $B(\mathscr{H})_1$, over a separable Hilbert space $\mathscr{H}$. $B(\mathscr{H})_1^{\text{s.a.}}$ is a real Banach space and the density matrices are its positive, normalized ($\operatorname{Tr}[\,]=1$) elements.

(2) By a straightforward application of the min–max principle we can express $\rho(n)\equiv\Sigma_{i=1}^{n}\rho_i$ as follows:

$$\rho(n)=\sup_{\mathscr{H}_n}\operatorname{Tr}_{\mathscr{H}_n}\hat{\rho},$$

i.e., the trace is computed over a basis of an n-dimensional subspace of the Hilbert space $\mathscr{H}$.

(3) Important results stemming from the theory of Refs. 2–4 are: (i) $\vdash$ is a partial order among the density matrices giving rise to equivalence classes of equally mixed states (there are, of course, density matrices whose eigenvalues cannot be compared in the above sense); (ii) $\operatorname{Tr} f(\hat{\rho})\geqslant\operatorname{Tr} f(\hat{\sigma})$ for any concave function on $\mathbf{R}_+$ if and only if $\hat{\rho}\vdash\hat{\sigma}$, $\hat{\rho}$ and $\hat{\sigma}$ two density matrices [not only the von Neumann entropy $S(\hat{\rho})=-\operatorname{Tr}\hat{\rho}\ln\hat{\rho}$ is bigger than $S(\hat{\sigma})$ but also all the so-called α entropies[3] $S_\alpha(\hat{\rho})=[1/(1-\alpha)]\ln\operatorname{Tr}\hat{\rho}^\alpha$, $\alpha\in\mathbf{R}_+\setminus\{1\}$, increase going from $\hat{\sigma}$ to $\hat{\rho}$]; (iii) $\hat{\rho}\vdash\hat{\sigma}$ if and only if

$$\hat{\rho}=\text{weak}\lim_{\alpha}\sum_i\lambda_{i\alpha}U_{i\alpha}^{\dagger}\hat{\sigma}U_{i\alpha},$$

$U_{i\alpha}$ unitary operators $\forall i,\alpha$; $0\leqslant\lambda_{i\alpha}\leqslant1$, $\Sigma_i\lambda_{i\alpha}=1$. [An example is provided by the time-averaged density matrix

$$\bar{\hat{\rho}}=\frac{1}{T}\int_0^T dt\exp\left(-\frac{i}{\hbar}Ht\right)\hat{\rho}\exp\left(\frac{i}{\hbar}Ht\right)$$

which is more mixed than $\hat{\rho}$, $\exp[-(i/\hbar)Ht]$ being the evolution operator for a given Hamiltonian H.]

The class of quantum dynamical semigroups we shall consider is the one that arises when the quantum system of interest is weakly interacting with an infinite reservoir.

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Under certain conditions on the form of the coupling and the kind of the chosen reservoir, the reduced evolution for the state $\hat{\rho}$ of the (open) system is Markoffian[7,8] and generated by

$$\partial_t \hat{\rho}_t = -i[\hat{H},\hat{\rho}_t] - \frac{1}{2}\sum_j \{B_j^\dagger B_j,\hat{\rho}_t\} + \sum_j B_j \hat{\rho}_t B_j^\dagger \equiv L[\hat{\rho}_t], \tag{2.3}$$

$B_j, B_j^\dagger, H = H^\dagger, \Sigma_j B_j^\dagger B_j \in B(\mathscr{H})$ (Banach space of bounded operators on $\mathscr{H}$).

Remark 2.4: The rhs of (2.3) is the most general expression for the generator $L[\cdot]$ of a norm-continuous semigroup $\{\gamma_t\}_{t\geqslant 0}$ of completely positive[9] contractions on the state space ($\gamma_t\hat{\rho} = \hat{\rho}_t$).[8,10] If the boundedness of the Hamiltonian, as it is often the case, is relaxed, then it could be proved that $L[\cdot]$ is the generator of a strongly continuous semigroup with respect to the trace norm:[7] (i) $\mathrm{Tr}\,\gamma_t\hat{\rho} = \mathrm{Tr}\,\hat{\rho}$ (probability preserving property); (ii) $\|\gamma_t\hat{\rho}\|_1 \leqslant \|\hat{\rho}\|_1$ ($\|\hat{\sigma}\|_1 = \mathrm{Tr}\sqrt{\hat{\sigma}^\dagger\hat{\sigma}}$); (iii) $\gamma_t \circ \gamma_s = \gamma_{t+s}$; $t, s \geqslant 0$ (semigroup property); (iv) γ_t is completely positive, $t \geqslant 0$; (v) $\|\gamma_t\hat{\rho} - \hat{\rho}\|_1 \overset{t\to 0^+}{\to} 0$ (instead of the stronger $\|\gamma_t - \mathbf{1}\| \overset{t\to 0^+}{\to} 0$).

Now we are in the position to claim the following proposition.

Proposition 2.5: If $T[\hat{\rho}] = \Sigma_j B_j \hat{\rho} B_j^\dagger$ is such that $T[\mathbf{1}] = \mathbf{1}$ as a map from $B(\mathscr{H})$ into $B(\mathscr{H})$ and $\Sigma_j B_j^\dagger B_j = \mathbf{1}$, then the semigroup generated by

$$L[\hat{\rho}] = -i[H,\hat{\rho}] - \hat{\rho} + T[\hat{\rho}] \tag{2.6}$$

is mixing enhancing.

Remark 2.7: The condition on $T[\cdot]$ is fulfilled by choosing, for instance, $B_j = B_j^\dagger$ with $\Sigma_j B_j^2 = 1$, e.g., a complete set of orthogonal projectors.

Proof: According to Remark 2.4 $L[\cdot]$ generates a semigroup $\{\gamma_t\}_{t\geqslant 0}$ of completely positive, trace preserving contractions on $B(\mathscr{H})_1^{s.a}$. Moreover, $T[\mathbf{1}] = \mathbf{1}$, $\forall t \geqslant 0$ when γ_t is extended on $B(\mathscr{H})^{s.a}$.

In the duality given by the trace we make correspond to γ_t a dual map $\gamma_t^*: B(\mathscr{H})^{s.a} \to B(\mathscr{H})^{s.a}$ which is in turn completely positive, identity, and trace preserving.

Given an initial density matrix $\hat{\rho}$, set $\hat{\rho}_t \equiv \gamma_t[\hat{\rho}]$ and let $t \geqslant 0$ be $s + \tau$ for $s, \tau \geqslant 0$. We now follow (Ref. 4, Chap. 2) and consider the family $F_N \subset B(\mathscr{H})^{s.a}$ of positive operators of rank N, bounded above by the identity. Recall now Remark 2.2.2 and note then $\gamma_t^*[F_N] \subseteq F_N$ so that $\forall N \geqslant 1$:

$$\rho_t(N) = \sup_{\mathscr{H}_N} \mathrm{Tr}_{\mathscr{H}_N} \gamma_\tau[\hat{\rho}_s] = \sup_{D\in F_N} \mathrm{Tr}\,\gamma_\tau^*[D]\hat{\rho}_s \leqslant \sup_{B\in F_N} \mathrm{Tr}\,B\hat{\rho}_s = \rho_s(N)\rangle$$

and hence: $\hat{\rho}_t \succ \hat{\rho}_s$ if $t \geqslant s \geqslant 0$ according to Definition 2.1.

Remark 2.8: We have not used the complete positivity of γ_t, but only the positivity which, together with $\mathrm{Tr}\,\gamma_t[\hat{\rho}] = \mathrm{tr}\,\hat{\rho}$ and $\gamma_t[\mathbf{1}] = \mathbf{1}$, characterizes the "doubly stochastic maps" (Ref. 4, Chap. 2). On the other hand, if we require $\{\gamma_t\}_{t\geqslant 0}$ to be a norm continuous semigroup of mixing enhancing, completely positive trace-preserving maps on $B(\mathscr{H})_1^{s.a}$, then γ_t must be doubly stochastic $\forall t \geqslant 0$ (Ref. 4, Chap. 2). Thus $\gamma_t[\mathbf{1}] = \mathbf{1}$ and, by Lindblad's theorem,[10] $L[\cdot]$ has the form (2.6).

The two simple examples reported in Ref. 1 serve to illustrate the following mechanism:

(1)

$$B(\mathscr{H})_1 \equiv B(\mathscr{H}) \equiv B(\mathbf{C}^2),$$

$$H = 0, \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = B^\dagger, \quad B^\dagger B = B^2 = \mathbf{1},$$

$$L[\hat{\rho}] = -\hat{\rho} + T[\hat{\rho}] = -\hat{\rho} + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\hat{\rho}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$T[\mathbf{1}] = \mathbf{1}.$$

Given the initial condition $\hat{\rho} = \begin{pmatrix} \rho & 0 \\ 0 & 1-\rho \end{pmatrix}$ the solution is

$$\hat{\rho}_t = \begin{pmatrix} \frac{1}{2} - \frac{1-2\rho}{2}e^{-2t} & 0 \\ 0 & \frac{1}{2} + \frac{1-2\rho}{2}e^{-2t} \end{pmatrix} = \begin{pmatrix} \rho_1(t) & 0 \\ 0 & \rho_2(t) \end{pmatrix}.$$

If $\rho > 1/2$ then $\rho_1(t) > \rho_2(t)\,\forall t \in [0, +\infty)$.

According to the notation introduced in Definition 2.1,

$$\rho_t(1) \equiv \rho_1(t) < \rho_1(s) \equiv \rho_s(1) < \rho \equiv \rho(1), \quad \forall 0 < s < t,$$

$$\rho_t(2) \equiv \rho_1(t) + \rho_2(t) = 1 = \rho_s(2) = \rho(2), \quad \forall 0 < s < t.$$

Therefore $\hat{\rho}_t \succ \hat{\rho}_s$ for any $t \geqslant s \geqslant 0$.

The smallest eigenvalue $\rho_2(t) = \frac{1}{2} + [(1-2\rho)/2]e^{-2t}$ keeps on increasing and $\rho_2(t)$ decreasing until, asymptotically, $\rho_1(\infty) = \rho_2(\infty) = 1/2$ corresponding to the most mixed state $\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and to the maximal entropy $S(\hat{\rho}_\infty) = \ln 2$.

(2)

$$B(\mathscr{H})_1 \equiv B(\mathscr{H}) \equiv B(\mathbf{C}^2),$$

$$H = 0, \quad B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},$$

$$B^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$$B^\dagger B \neq \mathbf{1}, \quad BB^\dagger \neq \mathbf{1},$$

$$L[\hat{\rho}_t] = -\frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}\hat{\rho}_t - \frac{1}{2}\hat{\rho}_t\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\hat{\rho}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = -\frac{1}{2}\{B^\dagger B,\hat{\rho}_t\} + B\hat{\rho}_t B^\dagger.$$

$T[\hat{\rho}_t] = B\hat{\rho}_t B^\dagger$ is such that $T[\mathbf{1}] \neq \mathbf{1}$.

Given the initial condition $\hat{\rho} = \begin{pmatrix} 1-\rho & 0 \\ 0 & \rho \end{pmatrix}$ the solution is

$$\hat{\rho}_t = \begin{pmatrix} 1-\rho e^{-t} & 0 \\ 0 & \rho e^{-t} \end{pmatrix} = \begin{pmatrix} \rho_1(t) & 0 \\ 0 & \rho_2(t) \end{pmatrix}.$$

If $\rho > 1/2$ then we have a crossing at $t_0 = \ln 2\rho > 0$.
For $0 \leqslant t \leqslant t_0 \rho_1(t) \leqslant \rho_2(t)$ and $0 \leqslant s \leqslant t$

$$\rho_t(1) \equiv \rho_2(t) = \rho e^{-t} \leqslant \rho e^{-s} = \rho_2(s) \equiv \rho_s(1) \leqslant \rho \equiv \rho(1).$$

Thus we have mixing enhancing in this time interval.
For $t \geqslant t_0 \rho_1(t) \geqslant \rho_2(t)$ and

$$\rho_t(1) \equiv \rho_1(t) = 1 - \rho e^{-t} \geqslant 1 - \rho e^{-t_0} = \tfrac{1}{2} \equiv \rho_{t_0}(1),$$

and we have the converse, namely, $\hat{\rho}_t$ gets ever less mixed than $\hat{\rho}_{t_0}$ for $t \geqslant t_0$ according to the fact that $\hat{\rho}_{t_0} = \frac{1}{2}\mathbf{1}$ is the most mixed state.
Asymptotically $\hat{\rho}_t$ reaches the least mixed state represented by the projector $\hat{\rho}_\infty = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$.

For $\rho < 1/2$ we have no crossing and $1 - \rho e^{-t} > \rho e^{-t}$ for any $t \geqslant 0$. Hence,

$$\rho_t(1) \equiv \rho_1(t) \geqslant \rho_1(s) \equiv \rho_s(1) \geqslant \rho(1), \quad \text{for any } t \geqslant s \geqslant 0$$

and the uncertainty inherent to the initial state $\hat{\rho}$ starts decreasing at $t = 0$.

This example shows that the conditions of Proposition 2.5 are, in a sense, optimal.

III. STRUCTURE OF THE SOLUTION AND INVESTIGATION OF SOME EXPLICIT MODELS

Now we want to consider a particular class of quantum dynamical semigroups that fulfill the conditions of Proposition 2.5. The purpose is exhibiting as explicitly as possible how mixing enhancing shows up when we are concerned with the solution of Eq. (2.3), namely, with the density matrix at time t, i.e., $\hat{\rho}_t$.

According to Remark 2.2.3.iii, we should expect indeed that $\hat{\rho}_t$ may be expressed by means of a linear convex combination of unitary transformations of the initial condition $\hat{\rho}$.

The semigroups at issue will be those generated by

$$L[\hat{\rho}_t] = -\frac{i}{\hbar}[\hat{H},\hat{\rho}_t] - \lambda\hat{\rho}_t + \lambda\left(\frac{1}{\hbar\sqrt{\alpha\pi}}\right)^3 \times \int_{\mathbf{R}^3} d\mathbf{p} \exp\left(-\frac{|\mathbf{p}|^2}{\alpha\hbar^2}\right) \times \exp\left(\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right)\hat{\rho}_t \exp\left(-\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right), \tag{3.1}$$

where $\hat{\mathbf{q}} \equiv (\hat{q}_1, \hat{q}_2, \hat{q}_3)$ is the three-dimensional position operator; λ is a characteristic frequency, and $1/\sqrt{\alpha}$ an intrinsic length of the model.

By comparing (3.1) with (2.3) we recognize that $T[\cdot] \equiv \Sigma_i B_i [\cdot] B_i^\dagger$ is replaced by

$$\left(\frac{1}{\hbar\sqrt{\alpha\pi}}\right)^3 \int_{\mathbf{R}^3} d\mathbf{p} \exp\left(-\frac{|\mathbf{p}|^2}{\alpha\hbar^2}\right) \times \exp\left(\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right)[\cdot]\exp\left(-\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right).$$

Furthermore, $\Sigma_i B_i^\dagger B_i$ now reads

$$\left(\frac{1}{\hbar\sqrt{\alpha\pi}}\right)^3 \int_{\mathbf{R}^3} d\mathbf{p} \exp\left(-\frac{|\mathbf{p}|^2}{\alpha\hbar^2}\right)\hat{\mathbf{1}} \equiv \hat{\mathbf{1}}$$

as well as $\Sigma_i B_i B_i^\dagger$.

Hence $T[\hat{\mathbf{1}}] = \hat{\mathbf{1}}$ and thus the conditions of Proposition 2.5 are met by generators of the above type where the dissipative part $L_d[\hat{\rho}_t] = -\lambda\hat{\rho}_t + \lambda T[\hat{\rho}_t]$ is once and for all fixed, whereas all the possible Hamiltonians can be considered.

This nonunitary modification of the usual Schrödinger evolution, given by $-(i/\hbar)[\hat{H},\cdot]$, constitutes the corner stone of the so-called "quantum mechanics with spontaneous localization" (QMSL),[6] which turned out to be a successful attempt to lay down a reasonable dynamical way out of the puzzling situations connected with the quantum description of macrosystems, e.g., the pointers in the descriptions of the measurement process.[11]

The original equation at the basis of QMSL, as written down in Ref. 6, reads

$$\partial_t\hat{\rho}_t = -\frac{i}{\hbar}[H,\hat{\rho}_t] - \lambda\hat{\rho}_t + \lambda\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{+\infty} dx \times \exp\left(-\frac{\alpha}{2}(\hat{q}-x)^2\right)\hat{\rho}_t \exp\left(-\frac{\alpha}{2}(\hat{q}-x)^2\right) \tag{3.2}$$

for a single quantum particle living in one dimension. That the processes

$$T[\hat{\rho}_t] = \sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{+\infty} dx \times \exp\left(-\frac{\alpha}{2}(\hat{q}-x)^2\right)\hat{\rho}_t \exp\left(-\frac{\alpha}{2}(\hat{q}-x)^2\right)$$

that occur with mean frequency λ, do actually provide localizations of the system is easily seen as follows: since

$$\langle q|T[\hat{\rho}]|\bar{q}\rangle = \exp[-(\alpha/4)(q-\bar{q})^2]\langle q|\hat{\rho}|\bar{q}\rangle,$$

it is apparent that off diagonalities in the position representation pretending to survive beyond the intrinsic length $(\sqrt{\alpha})^{-1}$, are strongly damped by the exponential.
Explicit solutions of (3.2) have been worked out in the following two cases:

$\hat{H} = \hat{p}^2/2m$ (Ref. 6),

$$\langle q|\hat{\rho}_t|\bar{q}\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp\left(-\frac{i}{\hbar}xy\right) \times \exp\left(-\lambda t + \lambda\int_0^t ds \exp\left[-\frac{\alpha}{4}\left(\frac{ys}{m} - x\right)^2\right]\right) \cdot \langle q + x|\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\hat{\rho}\exp\left(\frac{i}{\hbar}\hat{H}t\right)|\bar{q} + x\rangle, \tag{3.3}$$

$\hat{H} = \dfrac{\hat{p}^2}{2m} + \dfrac{m\omega^2}{2}\hat{q}^2$ (Ref. 12),

$$\langle q|\hat{\rho}_t|\bar{q}\rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \exp\left(-\frac{i}{\hbar}xy\right) \times \exp\left(-\lambda t + \lambda\int_0^t ds\right.$$

$$\times\exp\left[-\frac{\alpha}{4}\left(x\cos\omega t-\frac{y}{m\omega}\sin\omega t\right)^2\right]\Big)$$
$$\cdot\langle q+x\left|\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\hat{\rho}\exp\left(\frac{i}{\hbar}\hat{H}t\right)\right|\bar{q}+x\rangle. \tag{3.4}$$

Remarks 3.5: (1) Both solutions do reveal the presence of a damping factor quite explicitly. This, by itself, would be, of course, extremely dangerous if the parameters of the model could not be chosen such that the ordinary quantum description for a microsystem is affected only after enormous time. This is indeed the case, together with a surprising additive effect[6] which makes the frequency λ multiplied by N if we consider the modified quantum evolution of the center of mass of an N-particle system. An almost never felt damping effect for few particles becomes, on the contrary, heavily influencing macrosystems.

(2) Equation (3.1) is just the generalization of (3.2) to the three-dimensional case,[13] only involving a Fourier transform of a Gaussian on $\mathbf{R}^3$ in the expression for $T[\cdot]$.

As written in (3.1), it is, however, easier to recognize that (i) $T[\cdot]$ can be physically interpreted as a process kicking the system and changing its momentum by an amount $\mathbf{p}$ with a Gaussian probability. This meets classical explanation (in the free case) as a Markov process on the phase space with a stochastic kernel that leads to the same interpretation.[14] (ii) $T[\cdot]$ is a contraction on $B^{\text{s.a.}}(\mathscr{H})_1:\|T[\hat{\sigma}]\|_1\leqslant\|\hat{\sigma}\|_1$ and mixing enhancing owing to Remark 2.2.3.iii, without paying any reference to its complete positivity and to the fact that $T[\hat{\mathbf{1}}]=\hat{\mathbf{1}}$.

Proposition 3.6: The solution of Eqs. (3.1) (for any choice of Hamiltonian $\hat{H}$) can be expressed by means of trace-norm convergent series that actually agrees with Remark 2.2.3.iii: it is a linear convex combination (in an appropriate weak-limit) of unitary transformations of the initial $\hat{\rho}$.

Proof: By considering the equivalent integral equation,

$$\hat{\rho}_t=e^{-\lambda t}U(t)\hat{\rho}U(-t)+\lambda\int_0^t ds\,e^{-\lambda(t-s)}U(t-s)T[\hat{\rho}_s]U(s-t), \tag{3.7}$$

$U(t)=\exp[-(i/\hbar)\hat{H}t]$,

after iterating we end up with

$$\hat{\rho}_t=e^{-\lambda t}U(t)\sum_{k=0}^{\infty}\lambda^k\int_0^t ds_k\,\tau_{s_k}^k[\hat{\rho}]U(-t), \tag{3.8}$$

$$\int_0^t ds_0\,\tau_{s_0}^0[\hat{\rho}]\equiv\hat{\rho},$$

$$\tau_{s_1}^1[\hat{\rho}]=U(-s_1)T[U(s_1)\hat{\rho}U(-s_1)]U(s_1),$$

$$\tau_{s_k}^k[\hat{\rho}]=U(-s_k)\int_0^{s_k}ds_{k-1}\times T[U(s_k)\tau_{s_{k-1}}^{k-1}[\hat{\rho}]U(-s_k)]U(s_k).$$

Since $T[\cdot]$ is a contraction (see Remark 3.5.ii)

$$\|\tau_{s_k}^k[\hat{\rho}]\|_1\leqslant\int_0^{s_k}ds_{k-1}\|\tau_{s_k}^{k-1}[\hat{\rho}]\|_1\leqslant\cdots\leqslant\frac{[s_k]^{k-1}}{(k-1)!}\|\hat{\rho}\|_1,$$

hence the series in (3.8) turns out to converge with respect to trace norm. Let $\hat{\mathbf{q}}(t)$ indicate the position operator at time t: $\hat{\mathbf{q}}(t)=U(-t)\hat{\mathbf{q}}U(t)$, $W(\mathbf{a},\mathbf{b})$ the Weyl operator $\exp((i/\hbar)(\mathbf{a}\hat{\mathbf{p}}+\mathbf{b}\hat{\mathbf{q}}))$ and let $W_t(\mathbf{a},\mathbf{b})$ be $U(-t)W(\mathbf{a},\mathbf{b})U(t)=\exp\{(i/\hbar)[\mathbf{a}\hat{\mathbf{p}}(t)+\mathbf{b}\hat{\mathbf{q}}(t)]\}$, then

$$\tau_{s_k}^k[\hat{\rho}]=\int_0^{s_k}ds_{k-1}\cdots\int_0^{s_2}ds_1\;U(-s_k)T[U(s_k)T[\cdots U(-s_1)T[U(s_1)\hat{\rho}U(-s_1)]U(s_1)]\cdots]U(s_k)$$
$$=\left(\frac{1}{\hbar\sqrt{\alpha\pi}}\right)^{3k}\int_0^{s_k}\cdots\int_0^{s_2}\int_{\mathbf{R}^3}d\mathbf{p}_k\cdots\int_{\mathbf{R}^3}d\mathbf{p}_1\exp\left(-\sum_{i=1}^k\frac{|\mathbf{p}_i|^2}{\alpha\hbar^2}\right)$$
$$\cdot W_{s_k}(0,\mathbf{p}_k)W_{s_1}(0,\mathbf{p}_1)\hat{\rho}W_{s_1}^\dagger(0,\mathbf{p}_1)\cdots W_{s_k}^\dagger(0,\mathbf{p}_k).$$

Let $\mathbf{T}[\cdots]$ be the time ordering defined by

$$\mathbf{T}[W_{t_2}(0,\mathbf{p}_2)W_{t_1}(0,\mathbf{p}_1)\hat{\rho}W_{t_1}^\dagger(0,\mathbf{p}_1)W_{t_2}^\dagger(0,\mathbf{p}_2)]=\begin{cases}W_{t_2}(0,\mathbf{p}_2)\cdots W_{t_2}^\dagger(0,\mathbf{p}_2), & \text{if } t_2>t_1,\\ W_{t_1}(0,\mathbf{p}_1)\cdots W_{t_1}^\dagger(0,\mathbf{p}_1), & \text{if } t_1>t_2\end{cases},$$

and remark the symmetry of the Gaussian with respect to the momenta $\mathbf{p}_j$'s. Hence,

$$\int_0^t ds_k\,\tau_{s_k}^k[\hat{\rho}]=\left(\frac{1}{\hbar\sqrt{\alpha\pi}}\right)^{3k}\frac{1}{k!}\int_0^t ds_k\cdots\int_0^t ds_1\int_{\mathbf{R}^3}d\mathbf{p}_k\cdots\int_{\mathbf{R}^3}d\mathbf{p}_1\exp\left(-\sum_{i=1}^k\frac{|\mathbf{p}_i|^2}{\alpha\hbar^2}\right)$$
$$\cdot\mathbf{T}[W_{s_k}(0,\mathbf{p}_k)\cdots\hat{\rho}\cdots W_{s_k}^\dagger(0,\mathbf{p}_k)]$$

and, finally,

$$\hat{\rho}_t=e^{-\lambda t}U(t)\sum_{k=0}^{\infty}\frac{\lambda^k}{k!}\int_0^t ds_k\cdots\int_0^t ds_1\int_{\mathbf{R}^3}d\mathbf{p}_k\cdots\int_{\mathbf{R}^3}d\mathbf{p}_1\frac{\exp-\Sigma_{i=1}^k(|\mathbf{p}_i|^2/\alpha\hbar^2)}{(\hbar\sqrt{\alpha\pi})^{3k}}\cdot$$
$$\cdot\mathbf{T}[W_{s_k}(0,\mathbf{p}_k)\cdots\hat{\rho}\cdots W_{s_k}^\dagger(0,\mathbf{p}_k)]U(-t). \tag{3.9}$$

Remark 3.10: Although very complicated—the coefficients λ_i's in 2.2.3.iii depending now on discrete and continuous indices mixed together—it is nevertheless true that they are positive, normalized, and actually the weights of unitary transformations of the initial $\hat{\rho}$ as given by the time ordering $\mathbf{T}[\cdots\hat{\rho}\cdots]$ of the various Weyl operators.

A more transparent evidence of the mixing enhancing structure of the evolution can be obtained trying to connect the series (3.9) with the solutions in the cases (3.3) and (3.4).

The huge difficulties arising from noncommutativity in the time-ordered terms of the series can be overcome if the Weyl operators keep their form under the time evolution. Such a situation occurs when the Hamiltonian, being at most quadratic in the positions and momenta, gives rise to linear Heisenberg equations: free particle and harmonic oscillator are two simple examples, and in the Appendix it is shown how to go from the series (3.9) to the solutions (3.3) and (3.4). Linear equations of motion in the Heisenberg picture lead to solutions at time $t(\hat{\mathbf{q}}(t),\hat{\mathbf{p}}(t))$ which are linear combinations of the initial conditions $(\hat{\mathbf{q}},\hat{\mathbf{p}})$, agree with the classical solutions and involve only a redefinition of the parameters in passing from $W(\mathbf{a},\mathbf{b})$ to

$$
\begin{aligned}
&W_t(\mathbf{a},\mathbf{b}) \equiv U(-t)\,W(\mathbf{a},\mathbf{b})\,U(t) = W(\mathbf{a}(t),\mathbf{b}(t)),\\
&\hat{q}_i(t) = \sum_{j=1}^{3} \Omega_{ij}^1(t)\hat{q}_j + \Omega_{ij}^2(t)\hat{p}_j + F_i^1(t),\\
&\qquad i = 1,2,3,\\
&\hat{p}_i(t) = \sum_{j=1}^{3} \Omega_{ij}^3(t)\hat{q}_j + \Omega_{ij}^4(t)\hat{p}_j + F_i^2(t),\\
&\Omega(t) \equiv \begin{bmatrix} \Omega_{ij}^1(t), & \Omega_{ij}^2(t) \\ \Omega_{ij}^3(t), & \Omega_{ij}^4(t) \end{bmatrix}
\end{aligned}
\tag{3.11}
$$

being a symplectic 6×6 matrix,

$$\begin{bmatrix} F_i^1(t) \\ F_i^2(t) \end{bmatrix}$$

an inhomogeneous term, coming from analogs in the Heisenberg equations.

Following the result in the Appendix let us now make the ansatz that the solution of (3.1) is given by

$$
\begin{aligned}
\hat{\rho}_t = \frac{1}{(2\pi\hbar)^6}\int\int\int\int_{\mathbf{R}^3} d\mathbf{x}\,d\mathbf{y}\,d\boldsymbol{\xi}\,d\boldsymbol{\pi}\,\exp\left(-\frac{i}{\hbar}\mathbf{y}\boldsymbol{\xi}\right)\\
\times\exp\left(-\frac{i}{\hbar}\mathbf{x}\boldsymbol{\pi}\right)F(\lambda,\boldsymbol{\xi},\boldsymbol{\pi},t)\,W(\mathbf{x},\mathbf{y})\\
\times U(t)\hat{\rho}U(-t)\,W^{\dagger}(\mathbf{x},\mathbf{y}),
\end{aligned}
\tag{3.12}
$$

where the $\hat{H}$ in

$$U(t) = \exp[-(i/\hbar)Ht]$$

is at most quadratic. Using the cyclicity of the trace and the Weyl relations we have that a Weyl operator $W(\mathbf{a},\mathbf{b})$ evolves according to

$$\gamma_t^* W(\mathbf{a},\mathbf{b}) = F(\lambda,\mathbf{a},-\mathbf{b},t)\,U(-t)\,W(\mathbf{a},\mathbf{b})\,U(t), \tag{3.13}$$

which derives from the definition of "dual" evolution,

$$\operatorname{tr}\hat{\rho}\gamma_t^* W(\mathbf{a},\mathbf{b}) = \operatorname{Tr}\gamma_t\hat{\rho}W(\mathbf{a},\mathbf{b}),$$

for any ρ in $B(\mathscr{H})_1^{\text{s.a.}}$.

Also, $\gamma_t^* W(\mathbf{a},\mathbf{b})$ must satisfy the "dual" equation of motion [dual to (3.1)]

$$
\begin{aligned}
\partial_t\gamma_t^* W(\mathbf{a},\mathbf{b}) = \frac{i}{\hbar}\,[\hat{H},\gamma_t^* W(\mathbf{a},\mathbf{b})] - \lambda\gamma_t^* W(\mathbf{a},\mathbf{b})\\
+\lambda\int_{\mathbf{R}^3} d\mathbf{p}\,\frac{\exp-|\mathbf{p}|^2/\alpha\hbar^2}{(\hbar\sqrt{\alpha\pi})^3}\\
\times\exp\left(-\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right)\gamma_t^* W(\mathbf{a},\mathbf{b})\exp\left(\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right).
\end{aligned}
\tag{3.14}
$$

By means of the linear solutions (3.11) we obtain

$$
\begin{aligned}
&\exp\left(-\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right)\gamma_t^* W(\mathbf{a},\mathbf{b})\exp\left(\frac{i}{\hbar}\hat{\mathbf{q}}\mathbf{p}\right)\\
&\quad = F(\lambda,\mathbf{a},-\mathbf{b},t)\{W^{\dagger}(0,+\mathbf{p})\,U(-t)\,W(\mathbf{a},\mathbf{b})\,U(t)\,W(0,+\mathbf{p})\}\\
&\quad = F(\lambda,\mathbf{a},-\mathbf{b},t)\,U(-t)\,W^{\dagger}(\boldsymbol{\xi}(-t,0,+\mathbf{p}),\boldsymbol{\pi}(-t,0,+\mathbf{p}))\,W(\mathbf{a},\mathbf{b})\,W(\boldsymbol{\xi}(-t,0,+\mathbf{p}),\boldsymbol{\pi}(-t,0,+\mathbf{p}))U(t)\\
&\quad = F(\lambda,\mathbf{a},-\mathbf{b},t)\,U(-t)\,W(\mathbf{a},\mathbf{b})\,U(t)\exp\left\{\frac{i}{\hbar}\,[\mathbf{a}\boldsymbol{\pi}(-t,0,\mathbf{p}) - \mathbf{b}\boldsymbol{\xi}(-t,0,\mathbf{p})]\right\}
\end{aligned}
$$

where

$$
\begin{aligned}
&\xi_i(-t,0,\mathbf{p}) = \sum_{j=1}^{3}\Omega_{ji}^2(-t)p_j,\\
&\qquad\qquad i = 1,2,3.\\
&\pi_i(-t,0,\mathbf{p}) = \sum_{j=1}^{3}\Omega_{ji}^1(-t)p_j,
\end{aligned}
$$

Notice that the inhomogeneous terms give rise to phases that cancel each other.

Inserting the above result into (3.14) we continue to the following equation for the function $F(\cdots)$:

$$\partial_t F(\lambda,\mathbf{a},-\mathbf{b},t) = -\lambda F(\lambda,\mathbf{a},-\mathbf{b},t) + \lambda \exp(-(\alpha/4)|\xi(-t,\mathbf{a},-\mathbf{b})|^2) F(\lambda,\mathbf{a},-\mathbf{b},t), \tag{3.15}$$

$$\xi_i(-t,\mathbf{a},-\mathbf{b}) = \sum_{k=1}^{3} [\Omega^1_{ik}(-t)a_k - \Omega^2_{ik}(-t)b_k], \quad i=1,2,3.$$

With the initial condition $\gamma^*_{t=0} W(\mathbf{a},\mathbf{b}) = W(\mathbf{a},\mathbf{b})$ we get

$$F(\lambda,\mathbf{a},\mathbf{b},t) = \exp\left\{-\lambda t + \lambda \int_0^t ds \exp\left(-\frac{\alpha}{4}|\xi(-t,\mathbf{a},\mathbf{b})|^2\right)\right\}. \tag{3.16}$$

Remarks 3.17: (1) If $\hat{H} = \hat{p}^2/2m$ then

$$\Omega(t) = \begin{bmatrix} 1 & t/m \\ 0 & 1 \end{bmatrix}$$

and $\xi(-t,a,b) = a - bt/m$, if $\hat{H} = \hat{p}^2/2m + (m\omega^2/2)\hat{q}^2$ then

$$\Omega(t) = \begin{bmatrix} \cos\omega t & \sin\omega t/m\omega \\ -m\omega \sin\omega t & \cos\omega t \end{bmatrix}$$

and $\xi(-t,a,b) = a\cos\omega t - (b/m\omega)\sin\omega t$, in agreement with (3.3) and (3.4), respectively.

(2) The nonintegrability of the function $F(\cdots)$ with respect to the variables **a** and **b** implies that its Fourier transform in (3.12) has to be understood in the distributional sense, the test function being represented by

$$\langle\psi|W(\mathbf{x},\mathbf{y})U(t)\hat{\rho}U(-t)W^\dagger(\mathbf{x},\mathbf{y})|\psi\rangle$$

for some state $|\psi\rangle$ in the Hilbert space $\mathscr{H}$. The whole integral makes sense through a weak-limit procedure as well as the formal manipulations in the Appendix. Within this scheme the Fourier transform of the function $F(\lambda,\mathbf{a},\mathbf{b},t)$ appears to be the weight in a linear convex combination of the initial $\hat{\rho}$ transformed unitarily by means of the Weyl operators.

IV. CONCLUSIONS

We have given a sufficient condition under which a quantum dynamical semigroup does enhance the mixing of a quantum system in the sense of the ordering among density matrices. Mixing enhancing shows up explicitly in the structure of the solution for generators whose dissipative part has been chosen to be a Gaussian distributed kicking process changing the momentum of the single particle quantum system and leading to localization in position.

This behavior is even more evident if we look at the solutions of the modified quantum evolutions (3.3) and (3.4). They happen to be particular cases of a more general class of solvable equations of motion where the Hamiltonian is at most quadratic.

The structure of the solutions reveals a common behavior that leads to decaying of off-diagonal matrix elements in the position representation, together with general decreasing of information about the system. It is also clear that the linearity of the Heisenberg equations of motion and thus the equivalence of classical and quantum solutions, besides allowing us to solve the modified dynamics, characterizes the damping factor in the weight function. How far this is related to the classical limit in Ref. 14 would be a matter of subsequent investigation.

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APPENDIX: HARMONIC OSCILLATOR

Let us consider $\hat{H} = \hat{p}^2/2m + (m\omega^2/2)\hat{q}^2$ for which

$$\hat{q}_t = \hat{q}\cos\omega t + (\hat{p}/m\omega)\sin\omega t, \quad \hat{p}_t = \hat{p}\cos\omega t - m\omega\hat{q}\sin\omega t,$$

and

$$W_t(0,p) = U(-t)W(0,p)U(t) = \exp\left(\frac{i}{\hbar}p\hat{q}_t\right) = W\left(\frac{p}{m\omega}\sin\omega t, p\cos\omega t\right).$$

Using the Weyl relation we get

$$\mathbf{T}[W_{s_k}(0,p_k)\cdots W_{s_1}(0,p_1)\hat{\rho}W^\dagger_{s_1}(0,p_1)\cdots W^\dagger_{s_k}(0,p_k)] = W\left(\sum_{i=1}^k \frac{p_i}{m\omega}\sin\omega s_i, \sum_{i=1}^k p_i\cos\omega s_i\right)\hat{\rho}W^\dagger\left(\sum_{i=1}^k \frac{p_i}{m\omega}\sin\omega s_i, \sum_{i=1}^k p_i\cos\omega s_i\right).$$

Hence

$$\int_0^t ds_k \tau_{s_k}^k[\hat{\rho}] = \frac{1}{k!}\frac{1}{(\hbar\sqrt{\alpha\pi})^k}\int_0^t ds_k \cdots \int_0^t ds_1 \int_{-\infty}^{+\infty} dp_k \cdots \int_{-\infty}^{+\infty} dp_1 \exp\left(-\sum_{i=1}^k \frac{p_i^2}{\alpha\hbar^2}\right)$$
$$\cdot\frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left[-\frac{i}{\hbar}p\left(x - \sum_{i=1}^k \frac{p_i}{m\omega}\sin\omega s_i\right)\right].$$
$$\cdot\exp\left[-\frac{i}{\hbar}q\left(y - \sum_{i=1}^k p_i \cos\omega s_i\right)\right] W(x,y)\hat{\rho}W^\dagger(x,y)$$
$$= \frac{1}{k!}\frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left(-\frac{i}{\hbar}px\right)\exp\left(-\frac{i}{\hbar}qy\right)$$
$$\cdot\prod_{j=1}^k \left\{\int_0^t ds_j \frac{1}{\hbar\sqrt{\alpha\pi}}\int_{-\infty}^{+\infty} dp_j \exp\left(-\frac{p_j^2}{\alpha\hbar^2}\right)\exp\left(\frac{i}{\hbar}p_j\left[\frac{p}{m\omega}\sin\omega s_j + q\cos\omega s_j\right]\right)\right\}\cdot W(x,y)\hat{\rho}W^\dagger(x,y)$$
$$= \frac{1}{k!}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left(-\frac{i}{\hbar}px\right)\exp\left(-\frac{i}{\hbar}qy\right).$$
$$\cdot\left\{\int_0^t ds \exp\left(-\frac{\alpha}{4}\left[q\cos\omega s + \frac{p}{m\omega}\sin\omega s\right]^2\right)\right\}^k W(x,y)\hat{\rho}W^\dagger(x,y).$$

Finally,

$$\hat{\rho}_t = e^{-\lambda t}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left(-\frac{i}{\hbar}px\right)\exp\left(-\frac{i}{\hbar}qy\right)$$
$$\cdot\exp\left\{\lambda\int_0^t ds \exp\left(-\frac{\alpha}{4}\left[q\cos\omega s + \frac{p}{m\omega}\sin\omega s\right]^2\right)\right\} U(t)W(x,y)\hat{\rho}W^\dagger(x,y)U(-t).$$

The use being made of Dirac deltas, the exchange of integrals among themselves and with the sum are justified by going in a representation with suitable vector states in the Hilbert space $\mathscr{H}$ and by remarking the trace-norm convergence of the series (3.9).

Since

$$U(t)W(x,y)\hat{\rho}W^\dagger(x,y)U(-t) = W_{-t}(x,y)U(t)\hat{\rho}U(-t)W^\dagger_{-t}(x,y),$$

where

$$W_{-t}(x,y) = W[x\cos\omega t - (y/m\omega)\sin\omega t, y\cos\omega t + m\omega x\sin\omega t],$$

after a coordinate transformation, we end up with

$$\hat{\rho}_t = \frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left(-\frac{i}{\hbar}qy\right)\exp\left(-\frac{i}{\hbar}px\right)$$
$$\times\exp\left\{-\lambda t + \lambda\int_0^t ds \exp\left(-\frac{\alpha}{4}\left[q\cos\omega s - \frac{p}{m\omega}\sin\omega s\right]^2\right)\right\} W(x,y)U(t)\hat{\rho}U(-t)W^\dagger(x,y),$$

which agrees with (3.4) as we can see by working out $\langle q|\hat{\rho}_t|\hat{q}\rangle$. The weight function is now

$$\frac{1}{(2\pi\hbar)^2}\int_{-\infty}^{+\infty} dq \int_{-\infty}^{+\infty} dp \exp\left(-\frac{i}{\hbar}qy\right)\exp\left(-\frac{i}{\hbar}px\right)F(\lambda,q,p,t),$$
$$F(\lambda,q,p,t) = \exp\left\{-\lambda t + \lambda\int_0^t ds \exp\left[-\frac{\alpha}{4}\left(q\cos\omega s - \frac{p}{m\omega}\sin\omega s\right)\right]^2\right\},$$

and is to be understood in a distributional sense.

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On the complete system of observables in quantum mechanics

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This paper contains a series of remarks about the concept of Complete System of Observables (CSO) in quantum mechanics and a discussion of two definitions of CSO, one given by Jauch [Helv. Phys. Acta **33**, 711 (1960)] and the other by Prugovecki [Can. J. Phys. **47**, 1083 (1968)].

I. INTRODUCTION

As is well known, the concept of Complete System of Observables (CSO) was introduced in quantum mechanics by Dirac[1] based on rather heuristic considerations on the problem of assigning unambiguous elements of a Hilbert space to sets of measurements on a physical system. Dirac's formulation becomes rigorous only in a few cases, for instance, when the dimension of the Hilbert space in consideration is finite, in which a self-adjoint operator has real pure point spectrum.

In general, Dirac's formulation is not suitable in infinite-dimensional Hilbert spaces and a new definition is needed if the CSO concept is to be applicable in quantum mechanics; this problem was considered by Prugovecki[2] and Jauch[3] in the 1960s, but it seems that it has not been analyzed recently.

In this section we give the definitions of Prugovecki and Jauch. In Sec. II some ideas supporting these definitions are presented, as well as some physical aspects of the CSO concept. In Sec. III we analyze the relations between these definitions and we also show that one definition implies the other under a suitable assumption; such an assumption was presented in Ref. 4 but not in Ref. 2, although it should have been presented. In Sec. IV some remarks concerning the CSO concept are given.

From now on $\mathscr{H}$ will represent a separable complex Hilbert space and all measures in this work are σ-finite positive Borel measures on $\mathscr{R}^n$. If $(A_1,...,A_n)$ is a set of commuting self-adjoint operators in $\mathscr{H}$ (two self-adjoint operators commute iff their spectral families commute), the spectrum of A_i will be denoted by Λ_i and its spectral projections by $E^{A_i}(B)$, where B denotes any Borel set in $\mathscr{R}$.

As we consider here two definitions of CSO they will be distinguished as P-CSO and J-CSO, after Prugovecki and Jauch.

Definition 1 (Prugovecki[2]): The set $(A_1,...,A_n)$ of commuting self-adjoint operators in $\mathscr{H}$ constitutes a P-CSO iff there exists a unitary transformation $V:L^2_\mu(\Lambda)\to\mathscr{H}$, where $\Lambda=\Lambda_1\times\cdots\times\Lambda_n$ is the support of μ, such that the operators $V^{-1}A_iV$ are the multiplication operators

$$\mathrm{dom}(V^{-1}A_iV)$$
$$=\{\Psi\in L^2_\mu(\Lambda):\int_\Lambda x_i^2|\Psi(x)|^2\,d\mu(x)<\infty\},$$
$$(V^{-1}A_iV\Psi)(x)=x_i\Psi(x),\quad \Psi\in\mathrm{dom}(V^{-1}A_iV),$$
for $1\leqslant i\leqslant n$, $x=(x_1,...,x_n)$.

Now we turn our attention to Jauch's definition. If W is a set of operators in $\mathscr{H}$ its commutant W' is defined as the set of all bounded operators that commute with all the operators in W. If W contains only self-adjoint operators W', W'', W''',... are von Neumann algebras[4-6] (a set of continuous operators $\mathscr{U}$ is said to be a von Neumann algebra if $\mathscr{U}''=\mathscr{U}$); W'' is the smallest von Neumann algebra containing all the spectral projections of the operators in W and it is called the von Neumann algebra generated by W. A von Neumann algebra $\mathscr{U}$ is Abelian if $\mathscr{U}\subset\mathscr{U}'$ and, if, in addition, $\mathscr{U}'=\mathscr{U}$, $\mathscr{U}$ admits no Abelian extension and it is called maximal Abelian.

Definition 2 (Jauch[3]): The set $G=(A_1,...,A_n)$ of commuting self-adjoint operators in $\mathscr{H}$ constitute a J-CSO iff the von Neumann algebra generated by $G(G'')$ is maximal Abelian.

II. COMMENTS ON THE DEFINITIONS OF CSO

The existence of a CSO is tacitly made in quantum mechanics; this concept arises from the problem of assigning unambiguous elements of a Hilbert space to sets of measurements on a physical system, thus it is postulated the existence of a complete set of independent measurements that provide the maximum amount of information about the system. As each observable in quantum mechanics is represented by a self-adjoint operator in a Hilbert space, one arrives at the problem of characterizing a maximal set of self-adjoint operators.

The original formulation of the CSO concept given by Dirac[1] was developed based on properties of self-adjoint operators in finite-dimensional Hilbert spaces. The Hilbert spaces of quantum mechanics are, in general, infinite dimensional and some modifications are necessary to have this notion extended to the general case.

Jauch and Prugovecki redefined the concept of CSO in the finite-dimensional case in an equivalent way, which could be generalized to infinite-dimensional Hilbert spaces. Let us summarize the situation in the finite-dimensional case: According to Dirac's formulation a set $(F_1,...,F_n)$ of commuting self-adjoint operators forms a CSO in the finite-dimensional Hilbert space $\mathscr{K}$ if there is only one simultaneous eigenstate belonging to any set of eigenvalues. One can show that this definition is equivalent to any of the following assertions.

(a) (Refs. 2 and 4) There is a unitary mapping $V:L^2_\mu(\Lambda)\to\mathscr{K}$, such that

$$(V^{-1}F_iV\Psi)(x)=x_i\Psi(x),$$

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where μ is a finite measure and $x = (x_1,...,x_n)$.

(b) (Ref. 3) There is a vector $\xi \in \mathscr{K}$ such that every element $\eta \in \mathscr{K}$ can be represented in the form $\eta = p(F_1,...,F_n)\xi$ with some polynomial $p(F_1,...,F_n)$; Jauch[3] remarked that the set of such polynomials constitutes the von Neumann algebra generated by $(F_1,...,F_n)$ and this algebra is maximal Abelian.

The above assertions support the definitions of P-CSO and J-CSO. The definition of J-CSO is based on purely algebraic considerations and it also works for an arbitrary set of commuting self-adjoint operators.[3]

III. ON THE EQUIVALENCE OF J-CSO AND P-CSO

In this section we prove the equivalence (under certain assumptions) of the two CSO definitions given in Sec. I, but before this the definitions of P-CSO and J-CSO are related to the existence of cyclic vectors with respect to certain sets of operators.

Definition 3: Let $G = (A_1,...,A_n)$ be a set of commuting self-adjoint operators in $\mathscr{H}$. A $\xi \in \mathscr{H}$ is *P*-cyclic with respect to G iff $\xi \in \mathrm{dom}(p(A_1,...,A_n))$ for any polynomial $p(A_1,...,A_n)$ and the linear manifold spanned by all vectors of the form $p(A_1,...,A_n)\xi$ is dense in $\mathscr{H}$.

Definition 4: Let $G = (A_1,...,A_n)$ be a set of commuting self-adjoint operators in $\mathscr{H}$. A $\xi \in \mathscr{H}$ is *J*-cyclic with respect to G iff the linear manifold spanned by the vectors $(T\xi: T \in G'')$ is dense in $\mathscr{H}$.

Now we dwell on the explanation of an assumption needed for the validity of the "if part" of Lemma 1 below and of the spectral representation presented in Ref. 4.

If A:dom $A \to \mathscr{H}$ is self-adjoint and $\eta \in \mathrm{dom}\, A$ we have (by the Spectral Theorem[7])

$$\langle \eta | A\eta \rangle = \int_{\mathbf{R}} x \, dv_\eta^A(x), \tag{1}$$

where $v_\eta^A(B) = \langle \eta | E^A(B)\eta \rangle$ for any Borel set B in $\mathscr{R}$; if η is *J*-cyclic we can follow the arguments given in Ref. 4 and conclude that A acts as a multiplication by the independent variable in $L^2_{v_\eta^A}(\mathscr{R}^n)$.

Let $(A_1,...,A_n)$ be a set of n commuting self-adjoint operators in $\mathscr{H}$. There exists[4] a unique spectral measure S defined on the σ algebra generated by the Borel rectangles of the product space

$$\Lambda \equiv \Lambda_1 \times \cdots \times \Lambda_n,$$

such that

$$S(B_1 \times \cdots \times B_n) = E^{A_1}(B_1) \cdots E^{A_n}(B_n)$$

for any Borel rectangle $B_1 \times \cdots \times B_n$ in Λ.

For each $\eta \in \mathscr{H}$ we consider the σ-finite measure μ_η on the Borel sets of Λ, characterized by

$$\mu_\eta(B) = \langle \eta | S(B)\eta \rangle$$

for any Borel set B. For a convenient spectral representation of the elements of $(A_1,...,A_n)$ we should have[4]

$$\langle \xi | A_i \xi \rangle = \int_\Lambda x_i \, d\mu_\xi(x), \tag{2}$$

where $\xi \in \mathscr{H}$ is *J*-cyclic with respect to $(A_1,...,A_n)$ and $x = (x_1,...,x_n)$. [It will be shown that if assumption (3) holds, there exists a vector that is *P*-cyclic and *J*-cyclic with respect to $(A_1,...,A_n)$.]

If A_i is to be represented by the multiplication by x_i, we see that we should have[4]

$$\int_{\Lambda_i} x_i \, dv_\xi^{A_i}(x_i) = \int_\Lambda x_i \, d\mu_\xi(x), \tag{3}$$

and this will be supposed to be satisfied. It is worth noting the two following points.

(i) Assumption (3) is satisfied if μ_ξ is absolutely continuous with respect to the product measure (see Ref. 4),

$$v_\xi^{A_1} \times \cdots \times v_\xi^{A_n}.$$

(ii) In Ref. 2 relation (3) should be supposed to be satisfied for measure μ in Definition 1 [for instance, in Eq. (23)], and it is necessary for the validity of the "if part" of Lemma 1 below.

From now on we suppose that assumption (3) holds.

Lemma 1:[2] The set $(A_1,...,A_n)$ of commuting self-adjoint operators in $\mathscr{H}$ is a P-CSO iff there exists a vector *P*-cyclic with respect to $(A_1,...,A_n)$.

Lemma 2:[3] The set $(A_1,...,A_n)$ of commuting self-adjoint operators in $\mathscr{H}$ is a J-CSO iff there exists a *J*-cyclic vector with respect to $(A_1,...,A_n)$.

Suppose $(A_1,...,A_n)$ is a P-CSO. Let $\epsilon > 0$ and $\eta \in \mathscr{H}$ be given. By Lemma 1 there is a $\xi \in \mathscr{H}$ *P*-cyclic, so there is a polynomial $p(A_1,...,A_n)$ such that

$$\| p(A_1,...,A_n)\xi - \eta \| < \epsilon/2. \tag{4}$$

Let $I_1 CI_2 CI_3 C...$ measurable bounded sets in $\mathscr{R}^n$ such that

$$\mathbf{U}_{j=1}^{\infty} I_j = \mathscr{R}^n.$$

Using Lemma 1 and the representation of $(A_1,...,A_n)$ given in Definition 1 we have

$$\| \chi_{I_j}(A_1,...,A_n)p(A_1,...,A_n)\xi - p(A_1,...,A_n)\xi \|^2$$
$$= \int_\Lambda |\chi_{I_j}(x_1,...,x_n)p(x_1,...,x_n) - p(x_1,...,x_n)|^2 \, d\mu(x_1,...,x_n),$$

where $\Lambda = \Lambda_1 \times \cdots \times \Lambda_n$ and χ_I denotes the characteristic function of the set I. Since

$$|\chi_{I_j}(x_1,...,x_n)p(x_1,...,x_n) - p(x_1,...,x_n)|^2 \leqslant 4|p(x_1,...,x_n)|^2$$

and $|p(x_1,...,x_n)|^2$ is μ integrable we can apply the Dominate Convergence Theorem and conclude that there is a natural number k such that

$$\| \chi_{I_k}(A_1,...,A_n)p(A_1,...,A_n)\xi - p(A_1,...,A_n)\xi \| < \epsilon/2. \tag{5}$$

Combining Eqs. (4) and (5) we have

$$\| \chi_{I_k}(A_1,...,A_n)p(A_1,...,A_n)\xi - \eta \| < \epsilon.$$

Taking into account that the von Neumann algebra generated by $G = (A_1,...,A_n)$ consists precisely of the set of essentially bounded functions[4] of $(A_1,...,A_n)$, we see that $\chi_{I_k}(A_1,...,A_n)p(A_1,...,A_n)$ is an element of G''. Hence we conclude that ξ is a *J*-cyclic vector with respect to G, and according to Lemma 2, G is a J-CSO.

Now, suppose that $G = (A_1,...,A_n)$ is a J-CSO. Under assumption (3) Jauch and Misra[4] have shown that there is a

unique class $\mathscr{C}$ of equivalent measures on the σ algebra generated by the Borel rectangles of Λ, such that a measure $\rho\in\mathscr{C}$ if it has the form $\rho(B)=\langle\xi|S(B)\xi\rangle$ for some J-cyclic $\xi\in\mathscr{H}$; moreover, for any $\mu\in\mathscr{C}$, $\mathscr{H}$ is unitarily equivalent to $L^2_\mu(\Lambda)$ and A_i corresponds to the multiplication by x_i in $L^2_\mu(\Lambda)$. Hence G is also a P-CSO.

As a direct consequence of Lemmas 1 and 2, and the above paragraph, we have the following.

If η is a J-cyclic vector with respect to the J-CSO $G=(A_1,...,A_n)$, there is a P-cyclic vector ξ with respect to G, which is also a J-cyclic vector with respect to G. We have proved the following proposition.

Proposition 1 [under assumption (3)]: The set $G=(A_1,...,A_n)$ of commuting self-adjoint operators in $\mathscr{H}$ constitutes a J-CSO iff G is a P-CSO iff there is a $\xi\in\mathscr{H}$ that is J-cyclic and P-cyclic with respect to G.

IV. FURTHER REMARKS

In this section some remarks concerning the CSO concept are presented.

(i) The definition of J-CSO works for an arbitrary set of commuting self-adjoint operators,[3] as well as Lemma 2; but it does not seem to exist examples in quantum mechanics in which an infinite number of observables is necessary to constitute a CSO.

(ii) Assumption (3) is not necessary for the proof of Lemma 2.

(iii) Now we prove that if $(A_1,...,A_n)$ constitute a J-CSO and/or a P-CSO, then any other observable that commutes with $A_1,...,A_n$ is a function of $A_1,...,A_n$.

Proposition 2 [under assumption (3)]: Let $(A_1,...,A_n)$ be a J-CSO and/or a P-CSO. If T is a self-adjoint operator in $\mathscr{H}$ that commutes with $A_1,...,A_n$, then there exists a function f such that $T=f(A_1,...,A_n)$.

Proof: Suppose, to begin with, that T is bounded. By Proposition 1; there exists a P-cyclic vector ξ with respect to $(A_1,...,A_n)$. Thus there is a sequence of polynomials $(p_j(A_1,...,A_n))$ such that

$$p_j(A_1,...,A_n)\xi\to T\xi,\quad j\to\infty.$$

Since

$$\|p_j(A_1,...,A_n)\|^2=\int_\Lambda |p_j(x)|^2\,d\mu_\xi(x),$$

where $x=(x_1,...,x_n)$, it follows that $(p_j(x))$ is a Cauchy sequence in $L^2_{\mu_\xi}(\Lambda)$, and by the Riesz–Fischer Theorem there exists a $g\in L^2_{\mu_\xi}(\Lambda)$ such that

$$p_j\to g\quad\text{in } L^2_{\mu_\xi}(\Lambda).$$

Hence

$$\|p_j(A_1,...,A_n)\xi-g(A_1,...,A_n)\xi\|^2=\int_\Lambda |p_j(x)-g(x)|^2\,d\mu_\xi(x)\to 0,$$

and we have

$$p_j(A_1,...,A_n)\xi\to g(A_1,...,A_n)\xi,\quad j\to\infty.$$

Let $\eta\in\mathscr{H}$. There is a sequence of polynomials $(q_k(A_1,...,A_n))$ such that $(q_k(A_1,...,A_n)\xi)$ converges to η; since T is continuous and any function of commuting self-adjoint operators is a closed operator, it is clear that

$$Tq_k(A_1,...,A_n)\xi\to T\eta$$

and

$$\begin{aligned}g(A_1,...,A_n)q_k(A_1,...,A_n)\xi&=q_k(A_1,...,A_n)g(A_1,...,A_n)\xi\\&=q_k(A_1,...,A_n)T\xi\\&=Tq_k(A_1,...,A_n)\xi;\end{aligned}$$

hence we have $\eta\in\mathrm{dom}(g(A_1,...,A_n))$ and

$$g(A_1,...,A_n)q_k(A_1,...,A_n)\xi\to g(A_1,...,A_n)\eta;\quad k\to\infty;$$

therefore

$$T=g(A_1,...,A_n).$$

Finally, let T be an unbounded self-adjoint operator and $(E^T_y;y\in R)$ its spectral family. According to the above result, for each $y\in R$ there is a function f_y such that

$$E^T_y=f_y(A_1,...,A_n).$$

Since $(f_y;y\in R)$ characterizes uniquely[7] the operator T we may define the function

$$\begin{aligned}f(A_1,...,A_n)&\equiv\int y\,d_y[f_y(A_1,...,A_n)]\\&=\int y\,d_y[E^T_y]=T.\end{aligned}$$

(iv) Proposition 2 gives us a pleasant result from the physical point of view and justifies the word "complete" in the expression CSO; in fact, the result of Proposition 2 was considered by Mackey[8] as a convenient definition of CSO.

(v) Suppose the position operators $Q_1,...,Q_n$ of a quantum system in $\mathbf{R}^n$ constitute a J-CSO and/or a P-CSO, then $Q_1,...,Q_n$ are represented by the multiplication by $x_1,...,x_n$, respectively, in L^2_μ for some finite measure μ. If the momentum operators are defined as the generators of the translations

$$\mathbf{U}_{t_1,...,t_n}\Psi(x_1,...,x_n)=\Psi(x_1-t_1,...,x_n-t_n),$$

$\Psi\in L^2_\mu$, we have to assume that $U_{t_1,...,t_n}$ are unitary operators, since the momenta are observables (by The Stone Theorem[7]); hence the sets of μ measure zero must be translation invariant, which implies that μ is equivalent to the Lebesgue measure. Therefore μ and the Lebesgue measure are in the class $\mathscr{C}$ mentioned in Sec. III, so we can take the Hilbert space of the quantum system as $L^2(\mathscr{R}^n)$, with the Lebesgue measure, and $Q_1,...,Q_n$ as the multiplication by $x_1,...,x_n$, respectively; of course, this is the usual framework of the textbooks on quantum mechanics (also see Ref. 8).

(vi) As a final remark, we observe that in the case that a single operator A is a J-CSO and/or a P-CSO, Eq. (3) is always satisfied and Definition 1 express the so-called "canonical form" of the self-adjoint operator A.[7] Jauch and Misra[4] have announced examples where Eq. (3) is not satisfied.

V. CONCLUSION

We have discussed the concept of CSO in quantum mechanics from the mathematical and physical points of view;

special attention was given to the definitions and results of Jauch and Prugovecki. Many results obtained here were improvements of previous results and remarks given by other authors, but here it was possible to collect them together. An assumption made in this work was identity (3), and if identity (3) holds it was possible to prove the equivalence of J-CSO and P-CSO; we could think of identity (3) as a condition of independence of the operators in the CSO.

From the practical view, remark (v) in Sec. IV is outstanding, but it seems necessary to do analogous studies when other sets of operators are supposed to constitute a CSO, particularly sets containing the energy operator; in our opinion, there are physical aspects of the CSO concept not explored yet.

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Applications of the differentiability of eigenvectors and eigenvalues to a perturbed harmonic oscillator

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The potential interaction $\lambda x^2/(1+gx^2)$, $g>0$, of the harmonic oscillator $H_0 = -d^2/dx^2 + x^2$ considered as an operator in the space $L_2(-\infty, \infty)$ is bounded. This together with the nondegeneracy of the eigenvalues implies that the eigenvectors of the perturbed harmonic oscillator as functions of the parameters λ and g are strongly differentiable. The eigenvalues are therefore differentiable functions for every real λ and every real $g>0$. In particular, the first eigenvalue $E_1(\lambda)$ as a function of λ is strictly concave ($E_1''(\lambda)<0$). This paper, exploiting the above properties, aims at several inequalities for the eigenvalues of $H_0 + \lambda x^2/(1+gx^2)$, $g>0$. Emphasis is given to the inequality that follows from the strict concavity of the function $E_1(\lambda)$.

I. INTRODUCTION

A great amount of work has been devoted in the last few years to the investigation of the eigenvalues of the perturbed harmonic oscillator:

$$\left(-\frac{d^2}{dx^2} + x^2 + \frac{\lambda x^2}{1+gx^2}\right)\psi = E\psi; \quad \lambda>0, \quad g>0. \tag{1.1}$$

See Ref. 1 and the references therein.

A significant approximate relation for all eigenvalues E_n, $n\geqslant 0$, has been found in Ref. 2 for sufficiently small values of λ/g. This relation is

$$E_n \simeq 2n+1+\frac{1}{2}\frac{\lambda}{g} - \frac{\lambda}{g}(\sqrt{\pi}2^n n!)^{-1} I_n, \tag{1.2}$$

where

$$I_n = \int_0^\infty \exp(-x^2) H_n^2(x) \frac{1-gx^2}{1+gx^2}\,dx, \tag{1.3}$$

with $n=0, 1, 2,\ldots$ and $H_n(x)$ the Hermite polynomial of degree n.

The above approximation scheme, however, does not say how small are the values of λ/g for which (1.2) holds, and also, it is not apparent whether the approximation taken from (1.2) approximates the true eigenvalues from below or from above.

In this paper, we prove that for the first eigenvalue relation (1.2) is a strict inequality. In fact it is an upper bound and holds for every $\lambda>0$ and $g>0$. This has been achieved by proving that the first eigenvalue is a strictly concave function of λ in the interval $[0,\infty)$. The method we follow is based on the fact that the eigenfunctions of (1.1) are strongly differentiable functions with respect to λ in the space $L_2(-\infty,\infty)$.

The nonstrict concavity alone (without differentiability) can also be proved by the use of the minimum principle for the first eigenvalue.

The strict inequality in (1.2) is proved in Sec. III after giving some preliminaries in Sec. II. In Sec. IV a general comparison principle is proved from which several bounds for all the eigenvalues follow easily. In Sec. V numerical results are used for the estimation of the first eigenvalue $E_1(\lambda,g)$ for several values of λ and g.

II. PRELIMINARIES (ONE-PARAMETER PERTURBATION THEORY)

Suppose that $H(\nu)$ is a family of self-adjoint operators, bounded or unbounded in a separable Hilbert space H, depending on a real parameter ν in some open interval l_0 of the real axis. Suppose also that an isolated eigenvalue $E(\nu)$ of $H(\nu)$ exists for every ν in the open interval l_0 corresponding to the normalized eigenvector $x(\nu)$; $H(\nu)x(\nu) = E(\nu)x(\nu)$.

In Ref. 3, under the additional assumptions that

(i) $H(\nu)$ as a function of the real parameter ν is differentiable, with respect to the operator norm, for every ν in l_0, and the derivative

$$H'(\nu) = \frac{dH(\nu)}{d\nu}$$

is a uniformly bounded operator, i.e., $\|H'(\nu)\|\leqslant K<\infty$, on every compact subinterval of l_0; and

(ii) the eigenvalue $E(\nu)$ is simple (nondegenerate) for every ν in l_0, it has been proved that the corresponding eigenvector $x(\nu)$ as a function from l_0 into H, $x(\nu): l_0 \to H$, is strongly differentiable and the derivative $x'(\nu)$ is given by

$$x'(\nu) = -R(\nu)P(\nu)H'(\nu)x(\nu); \quad \|x(\nu)\| = 1, \tag{2.1}$$

where $P(\nu)$ is the orthogonal projection on $H\theta\{x(\nu)\}$ and $R(\nu)$ is the inverse of $H-E(\nu)I$, restricted on $H\theta\{x(\nu)\}$.

Now, from the relation

$$E(\nu) = \langle H(\nu)x(\nu), x(\nu)\rangle, \quad \|x(\nu)\| = 1,$$

it follows immediately that $E(\nu)$ is differentiable and the derivative $E'(\nu)$ is given by

$$E'(\nu) = \langle H'(\nu)x(\nu), x(\nu)\rangle, \quad \|x(\nu)\| = 1, \tag{2.2}$$

because $H(\nu)$ is self-adjoint.

The relation (2.2) is called in quantum chemistry a Hellman–Feynman theorem and it was known formally many years ago.[4] Formally, it was also known the relation

$$\frac{d^2E_1(\nu)}{d\nu^2} \leqslant \langle H''(\nu)x_1(\nu), x_1(\nu)\rangle, \tag{2.3}$$

for the first eigenvalue $E_1(\nu)$ in case where $H(\nu)$ is unbounded,[5] and the relation

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$$\frac{d^2E_1(\nu)}{d\nu^2} \geqslant \langle H''(\nu)x_1(\nu),x_1(\nu)\rangle , \tag{2.4}$$

for the last eigenvalue $E_1(\nu)$ in the case where $H(\nu)$ is bounded. See Ref. 3 for rigorous proofs.

Moreover, in the case where $H(\nu)$ has, for every ν in I_0, a complete orthonormal system of eigenvectors $x_n(\nu)$, $n = 1,2,...$, which correspond to the simple (nondegenerate) eigenvalues $E_n(\nu)$, one has from the above relations (2.1) and (2.2) the expression[3]

$$\frac{d^2E_k(\nu)}{d\nu^2} = \langle H''(\nu)x_k(\nu),x_k(\nu)\rangle - 2\sum_{\substack{n=1\\ n\neq k}}^{\infty} \frac{1}{E_n(\nu)-E_k(\nu)} \times |\langle H'(\nu)x_k(\nu),x_n(\nu)\rangle|^2 , \tag{2.5}$$

from which one obtains the so-called curvature theorems (2.3) and (2.4) for the first and the last eigenvalue, respectively. In Ref. 3 has been proved something more, that in the case where $H'(\nu)$ has purely continuous spectrum the strict inequalities in (2.3) and (2.4) hold.

We now consider the particular case of the operator $H(\nu)$ in which we are now interested:

$$H(\nu) = H_0 + \nu A, \quad H'(\nu) = A, \quad H''(\nu) = 0, \quad 0 \leqslant \nu \leqslant 1 . \tag{2.6}$$

In (2.6) H_0 is a self-adjoint operator with a complete orthonormal set of eigenvectors e_n, $n = 1, 2,...$, corresponding to the eigenvalues $c_1 < c_2 < c_3 < \cdots < c_n \to \infty$, and A is a bounded self-adjoint operator.

From the above we conclude the following.

The first eigenvalue $E_1(\nu)$ of the operator $H_0 + \nu A$ is strictly concave, i.e.,

$$\frac{d^2E_1(\nu)}{d\nu^2} < 0, \quad \nu \geqslant 0 , \tag{2.7}$$

when A has no eigenvalues. Note that strong differentiability of the eigenvectors $x_n(\nu)$, $n \geqslant 1$, implies weak continuity and this, together with the simplicity (nondegeneracy) of eigenvalues, leads to the fact that the variation of the parameter ν does not change the order of the eigenvalues

$$0 < E_1(\nu) < E_2(\nu) < \cdots < E_n(\nu) < \cdots .$$

Indeed, $E_1(\nu) < E_2(\nu)$ and $E_1(\mu) \geqslant E_2(\mu)$, $\mu > \nu$, implies that there exists a number ξ between ν and μ such that $E_1(\xi) = E_2(\xi)$. But for μ near ξ, $E_1(\mu) \neq E_2(\mu)$. This means that

$$\langle x_1(\mu),x_2(\mu)\rangle = 0 ,$$

and for $\mu \to \xi$,

$$\langle x_1(\xi),x_2(\xi)\rangle = 0 ,$$

contrary to the degeneracy of the eigenvalues. Thus $E_n(\nu)$ remains the nth eigenvalue for all ν. Also we have that $E_n(0) = c_n$ and $x_n(0) = e_n$. From (2.7) and (2.2) we obtain

$$\frac{dE_1(\nu)}{d\nu} < \frac{dE_1(0)}{d\nu} = \langle Ae_1,e_1\rangle , \tag{2.8}$$

so that for the first eigenvalue $E_1(\nu)$ of $H_0 + \nu A$ we have

$$E_1(\nu) < c_1 + \nu\langle Ae_1,e_1\rangle . \tag{2.9}$$

Then the first eigenvalue $E_1(1)$ of $H_0 + A$ satisfies the inequality

$$E_1(1) = E_1 < c_1 + \langle Ae_1,e_1\rangle . \tag{2.10}$$

Note that relation (2.10) says something more than the infimum principle:

$$E_1 = \inf_{\substack{f\in H\\ f\neq 0}} \langle (H_0 + A)f,f\rangle / \langle f,f\rangle \leqslant \langle (H_0 + A)e_1,e_1\rangle = c_1 + \langle Ae_1,e_1\rangle .$$

III. THE UPPER BOUND ON THE FIRST EIGENVALUE $E_1(\lambda)$

The one-dimensional Schrödinger equation

$$\left[-\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x) , \tag{3.1}$$

with an interaction of the type

$$V(x) = x^2 + \lambda x^2/(1 + gx^2), \quad g > 0, \quad \lambda > 0 , \tag{3.2}$$

takes exactly the form of an eigenvalue equation of the operator $H_0 + \lambda A$,

$$H(\lambda) = H_0 + \lambda A = H_0 + \lambda\,[x^2/(1 + gx^2)] , \tag{3.3}$$
$$H(\lambda)x_n(\lambda) = E_n(\lambda)x_n(\lambda) ,$$

considered here as a function of the potential parameter λ. Here, H_0 is taken as the harmonic oscillator operator

$$H_0 = -\frac{d^2}{dx^2} + x^2; \quad H_0e_n(x) = (2n-1)e_n(x); \quad n = 1,2... ,$$

with

$$e_n(x) = \left[\frac{1}{2^{n-1}(n-1)!\sqrt{\pi}}\right]^{1/2} e^{-x^2/2}H_{n-1}(x) \tag{3.4}$$

the corresponding normalized eigenfunctions, and A as the perturbation operator

$$A:\ Af(x) = [x^2/(1 + gx^2)]\,f(x) \tag{3.5}$$

in the space $L_2(-\infty,\infty)$. This is the case of the above considered particular form of the operator $H(\nu)$; $H(\nu) = H_0 + \nu A$, Eq. (2.6)

Now, assumption (i) is satisfied because the operator A in (3.5) is a bounded operator on $L_2(-\infty,\infty)$. Assumption (ii) is also satisfied for all eigenvalues $E_n(\lambda)$ in the case of the one-dimensional Schrödiner equation.

Chaudhuri and Mukherjee[2] in their study of the problem (3.3), in order to obtain the energy eigenvalues, have developed a simple approximation scheme only for small values of $k = \lambda/g$ and have been led to

$$E_n(k) \simeq 2n - 1 + \tfrac{1}{2}k - k\,[\sqrt{\pi}2^{n-1}(n-1)!]^{-1}I_{n-1} , \tag{3.6}$$

where

$$I_{n-1} = \int_0^{\infty} \exp(-x^2)H_{n-1}^2(x)\,\frac{1-gx^2}{1+gx^2}\,dx, \tag{3.7}$$

with $n = 1, 2,...$ and $H_n(x)$ is a Hermite polynomial of degree n.

Proposition 1: The relation (3.6) is a strict upper bound for the first eigenvalue $E_1(\lambda)$ for every $k=\lambda/g$ and can be expressed as follows:

$$E_1(\lambda)<1+\frac{\lambda}{g}\left[1-\pi^{1/2}g^{-1/2}e^{1/g}\left(1-\operatorname{erf}\frac{1}{\sqrt{g}}\right)\right]. \tag{3.8}$$

Proof: The first eigenvalue $E_1(\lambda)$ of the operator $H_0+\lambda A$ is strictly concave, i.e.,

$$\frac{d^2E_1(\lambda)}{d\lambda^2}<0; \tag{3.9}$$

because the operator A, defined by (3.5), has no eigenvalues. Since here $c_1=1$ and $e_1(x)=\pi^{-1/4}\cdot e^{-x^2/2}$ relation (2.9) leads to

$$E_1(\lambda)<1+\frac{\lambda}{g}\left[1-\pi^{-1/2}2\int_0^\infty\frac{e^{-x^2}}{1+gx^2}dx\right]. \tag{3.10}$$

Relation (3.8) follows by expressing the integral in (3.10) in terms of the error function.[6]

On the other hand, the relations (3.6) and (3.7) give for the first eigenvalue $E_1(\lambda)$ the following approximate expression:

$$E_1(\lambda)\simeq 1+\tfrac{1}{2}k-k\left[\sqrt{\pi}\right]^{-1}I_0$$
$$=1+\frac{1}{2}\frac{\lambda}{g}-\frac{\lambda}{g}\pi^{-1/2}\int_0^\infty\frac{1-gx^2}{1+gx^2}e^{-x^2}dx, \tag{3.11}$$

which after some manipulation can take the form

$$E_1(\lambda)\simeq 1+\frac{\lambda}{g}\left[1-\pi^{-1/2}2\int_0^\infty\frac{e^{-x^2}}{1+gx^2}dx\right]. \tag{3.12}$$

This shows that Chaudhuri and Mukherjee's relation (3.11) is in fact a strict inequality holding for every $k=\lambda/g$.

Remark 3.1: Inequality (3.8) follows from the strict concavity of the function $E_1(\lambda)$. In general, concavity or convexity is impossible for all eigenvalues of the parameter problem $(H_0+\lambda A)x(\lambda)=E(\lambda)x(\lambda)$. In fact, in a finite-dimensional space the first eigenvalue is concave and the last convex.[3] However, in infinite-dimensional spaces, there are cases where concavity holds for all eigenvalues, as we know from examples.

We believe that in the present case of the perturbed harmonic oscillator concavity holds for all eigenvalues and therefore the strict inequality in (3.6) holds for every $n=1,2,\ldots$.

IV. SOME MONOTONICITY PROPERTIES LEADING TO UPPER BOUNDS ON THE EIGENVALUES

The comparison principle we give below follows easily from those results of Ref. 3 that are briefly presented in Sec. II. This is given here in a general form and may be viewed as a generalization of a well-known comparison principle in the Sturm–Liouville eigenvalue problem.[7]

Proposition 2: Assume that the self-adjoint operator H_0 is bounded below with compact resolvent, so that the spectrum of H_0+A consist only of eigenvalues, for every bounded self-adjoint operator A. Assume also that the eigenvalues of H_0+A are nondegenerate and remain so if A is replaced by $a+\beta A$, $a\geqslant 0$, $\beta\geqslant 0$, $a^2+\beta^2\neq 0$. Then $A\leqslant B$ in the sense $\langle Af,f\rangle\leqslant\langle Bf,f\rangle$ implies $E_n(A)\leqslant E_n(B)$, where $E_n(A)$ and $E_n(B)$, $n\geqslant 1$, are, respectively, the eigenvalues of the problems $(H_0+A)f=Ef$, $(H_0+B)f=Ef$. Also the strict inequality holds, if $A<B$.

Proof: Consider the parameter eigenvalue problem

$$[H_0+(1-\nu)A+\nu B]x_n(\nu)=E_n(\nu)x_n(\nu),$$
$$0\leqslant\nu\leqslant 1, \tag{4.1}$$

so that $E_n(0)=E_n(A)$ and $E_n(1)=E_n(B)$, $n\geqslant 1$. From (2.2) we obtain

$$\frac{dE_n(\nu)}{d\nu}=\langle(B-A)x_n(\nu),x_n(\nu)\rangle\geqslant 0.$$

Thus

$$E_n(1)\geqslant E_n(0)\quad\text{or}\quad E_n(A)\leqslant E_n(B). \tag{4.2}$$

Applying this proposition to the eigenvalue problem (3.3) we obtain the following results:

(1) for every $\lambda>0$ and $g>0$ the eigenvalues $E_n(\lambda,g)$ of (3.3) satisfy the inequality

$$E_n(\lambda,g)<(2n-1)\sqrt{1+\lambda},\quad n\geqslant 1,\quad \lambda>0,\quad g>0. \tag{4.3}$$

This follows by comparing the interaction in (3.3) with the interaction $\lambda x^2(g=0)$ and is appropriate for every λ and small g, because for $g=0$ the equality holds.

(2) The eigenvalues $E_n(\lambda,g)$, for fixed λ, decrease as g increases and for fixed g increase with λ.

(3) For every λ and $g\neq 0$

$$E_n(\lambda,g)<2n-1+\lambda/g,\quad n\geqslant 1. \tag{4.4}$$

This follows because

$$\frac{\lambda x^2}{1+gx^2}=\frac{\lambda}{g}\frac{gx^2}{1+gx^2}<\frac{\lambda}{g}.$$

Note that the inequalities (4.3) and (4.4) are well known.[8]

V. NUMERICAL RESULTS

In Table I the upper bounds for the first eigenvalue $E_1(\lambda)$ have been determined from the inequality (3.8) which is in fact relation (3.10) expressed in terms of the error function. The numerical results are almost the same as those found in Ref. 2 by using a different expression of the integral in the right hand of (3.10).

Table II compares the upper bounds given by (3.8) for several values of λ and g with the upper bounds obtained in

TABLE I. Upper bounds for the first eigenvalue.

g	Upper bounds of Ref. 2	Upper bounds given by (3.8)
0.5	$1+0.314\,5246\lambda$	$1+0.314\,6656\,98\lambda$
1	$1+0.242\,1296\lambda$	$1+0.242\,1278\,48\lambda$
2	$1+0.172\,1604\lambda$	$1+0.172\,1602\,21\lambda$
5	$1+0.097\,9383\lambda$	$1+0.097\,9382\,51\lambda$
10	$1+0.059\,4434\lambda$	$1+0.059\,4434\,92\lambda$
20	$1+0.034\,3377\lambda$	$1+0.034\,3373\,26\lambda$
100	$1+0.008\,411\lambda$	$1+0.008\,4110\,713\lambda$
500	$1+0.001\,8451\lambda$	$1+0.001\,8491\,602\lambda$

TABLE II. Comparison of the upper bounds given by (3.8).

$g=0.5$			
$\lambda=0.1$	1.031 21	1.031 466 569	0.000 256 569
$\lambda=0.2$	1.061 96	1.062 933 139	0.000 973 139
$\lambda=0.5$	1.151 56	1.157 332 849	0.005 772 849
$\lambda=1$	1.292 95	1.314 665 698	0.021 715 698
$\lambda=2$	1.551 04	1.629 331 396	0.078 291 396
$\lambda=5$	2.192 11	2.573 328 49	0.381 218 49
$\lambda=10$	3.016 85	4.146 656 98	1.129 806 98
$\lambda=20$	4.255 06	7.293 313 96	3.038 253 96
$\lambda=50$	6.792 78	16.733 284 9	9.940 504 9
$\lambda=100$	9.692 15	32.466 569 8	22.774 419 8
$g=1$			
$\lambda=0.1$	1.024 10	1.024 212 784	0.000 112 784
$\lambda=0.2$	1.048 01	1.048 425 569	0.000 415 569
$\lambda=0.5$	1.118 54	1.121 063 924	0.002 523 924
$\lambda=1$	1.232 35	1.242 127 848	0.009 777 848
$\lambda=2$	1.447 32	1.484 255 696	0.036 935 696
$\lambda=5$	2.013 00	2.210 639 24	0.197 639 24
$\lambda=10$	2.782 33	3.421 278 48	0.638 948 48
$\lambda=20$	3.977 69	5.842 556 96	1.864 866 96
$\lambda=50$	6.478 11	13.106 392 4	6.628 282 4
$\lambda=100$	9.359 4	25.212 784 8	15.853 384 8
$g=2$			
$\lambda=0.1$	1.017 18	1.017 216 022	0.000 036 022
$\lambda=0.2$	1.034 29	1.034 432 044	0.000 142 044
$\lambda=0.5$	1.085 19	1.086 080 11	0.000 890 11
$\lambda=1$	1.168 67	1.172 160 221	0.003 490 221
$\lambda=2$	1.330 72	1.344 320 442	0.013 600 442
$\lambda=5$	1.782 13	1.860 801 105	0.078 671 105
$\lambda=10$	2.442 50	2.721 602 21	0.279 102 21
$\lambda=20$	3.534 92	4.443 204 42	0.908 284 42
$\lambda=50$	5.931 98	9.608 011 05	3.676 031 05
$\lambda=100$	8.758 2	18.216 022 1	9.457 822 1
$g=5$			
$\lambda=0.1$	1.009 78	1.009 793 825	0.000 013 825
$\lambda=0.2$	1.019 56	1.019 587 65	0.000 027 65
$\lambda=0.5$	1.048 86	1.048 969 125	0.000 109 125
$\lambda=1$	1.097 29	1.097 938 251	0.000 648 251
$\lambda=2$	1.193 31	1.195 876 502	0.002 566 502
$\lambda=5$	1.474 02	1.489 691 255	0.015 671 255
$\lambda=10$	1.918 90	1.979 382 51	0.060 482 51
$\lambda=20$	2.733 91	2.958 765 02	0.224 855 02
$\lambda=50$	4.755 70	5.896 912 55	1.141 212 55
$\lambda=100$	7.342 16	10.793 825 1	3.451 665 1
$g=10$			
$\lambda=0.1$	1.005 94	1.005 944 349	0.000 004 349
$\lambda=0.2$	1.011 88	1.011 888 698	0.000 008 698
$\lambda=0.5$	1.029 68	1.029 721 746	0.000 041 746
$\lambda=1$	1.059 29	1.059 443 492	0.000 153 492
$\lambda=2$	1.118 30	1.118 886 984	0.000 586 984
$\lambda=5$	1.293 58	1.297 217 46	0.003 637 46
$\lambda=10$	1.580 02	1.594 434 92	0.014 414 92
$\lambda=20$	2.132 43	2.188 869 84	0.056 439 84
$\lambda=50$	3.644 41	3.972 174 6	0.327 764 6
$\lambda=100$	5.794	6.944 349 2	1.150 349 2
$g=20$			
$\lambda=0.1$	1.003 43	1.003 433 732	0.000 003 732
$\lambda=0.2$	1.006 86	1.006 867 465	0.000 007 465
$\lambda=0.5$	1.017 16	1.017 168 663	0.000 008 663
$\lambda=1$	1.034 30	1.034 337 326	0.000 037 326
$\lambda=2$	1.068 55	1.068 674 652	0.000 124 652
$\lambda=5$	1.170 96	1.171 686 63	0.000 726 63
$\lambda=10$	1.340 47	1.343 373 26	0.002 903 26
$\lambda=20$	1.675 18	1.686 746 52	0.011 566 52
$\lambda=50$	2.645 47	2.716 866 3	0.071 396 3
$\lambda=100$	4.157	4.433 732 6	0.276 732 6

TABLE II. (*Continued.*)

$g=50$			
$\lambda=0.1$	1.001 56	1.001 569 622	0.000 009 622
$\lambda=0.2$	1.003 13	1.003 139 244	0.000 009 244
$\lambda=0.5$	1.007 84	1.007 848 11	0.000 008 11
$\lambda=1$	1.015 69	1.015 696 221	0.000 006 221
$\lambda=2$	1.031 38	1.031 392 442	0.000 012 442
$\lambda=5$	1.078 40	1.078 481 105	0.000 081 105
$\lambda=10$	1.156 67	1.156 962 21	0.000 292 21
$\lambda=20$	1.312.75	1.313 924 42	0.001 174 42
$\lambda=50$	1.777 48	1.784 811 05	0.007 331 05
$\lambda=100$	2.540 1	2.569 622 1	0.029 522 1
$g=100$			
$\lambda=0.1$	1.000 84	1.000 841 107	0.000 001 107
$\lambda=0.2$	1.001 68	1.001 682 214	0.000 002 214
$\lambda=0.5$	1.004 20	1.004 205 535	0.000 005 535
$\lambda=1$	1.008 41	1.008 411 071	0.000 001 071
$\lambda=2$	1.016 82	1.016 822 142	0.000 002 142
$\lambda=5$	1.042 04	1.042 055 356	0.000 015 356
$\lambda=10$	1.084 06	1.084 110 71	0.000 050 71
$\lambda=20$	1.168 03	1.168 221 42	0.000 191 42
$\lambda=50$	1.419 38	1.420 553 55	0.001 173 55
$\lambda=100$	1.836 4	1.841 107 1	0.004 707 1

Ref. 9 by the Ritz aproximation method and by using 30×30 and (for large values of g) 100×100 matrices. This table shows that the bounds found in Ref. 9 (first row of Table II) are better than the bounds given by (3.8) (second row of Table II). We see that for small values of the ratio λ/g the difference of these two bounds (third row of Table II) is not significant. More precisely it is of order $\alpha\times10^{-5}$ for $(\lambda/g)\leqslant0.1$, of order $\alpha\times10^{-4}$ for $(\lambda/g)\leqslant0.4$, of order $\alpha\times10^{-3}$ for $(\lambda/g)\leqslant1$ and of order $\alpha\times10^{-2}$ for $(\lambda/g)\leqslant4$, where $0<\alpha<10$.

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Factorizations of the S matrix[a)]

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The S matrix of the Schrödinger equation, regarded as a function on the real axis with values in the group of unitary operators $L^2(S^2) \mapsto L^2(S^2)$, where S^2 is the unit sphere in $\mathbb{R}^3$, is factorized in two different ways. One of these is a standard Wiener–Hopf factorization with respect to the real line. The other is the kind of factorization that defines the Jost function and which has been found to be a useful tool for the solution of the inverse scattering problem. A number of results are given that relate the two factorizations, their existence as well as the indices they give rise to. Some known theorems on the standard factorization lead to new results for the three-dimensional inverse scattering problem for the Schrödinger equation with a noncentral potential; in particular, a characterization of admissible S matrices is obtained.

I. INTRODUCTION

As is well known, the Jost function $f_l(k)$ plays an important role in scattering theory, and particularly in the inverse scattering problem at a fixed angular momentum, for the Schrödinger equation with a central potential. Under very general conditions this function is the continuous boundary value of an analytic function that is holomorphic in $\mathbb{C}^+$ and approaches unity at $|k| \to \infty$. Furthermore, it has a finite number of simple zeros on the positive imaginary axis at points $i\kappa_m$ if and only if $-\kappa_m^2$ is an eigenvalue of the radial Schrödinger equation of that particular angular momentum. The eigenvalue $S_l(k) = e^{2i\delta_l(k)}$ of the S matrix corresponding to angular momentum l can be factored as

$$S_l(k) = [1/f_l(k)]f_l(-k),$$

in which the first factor is meromorphic in the upper half-plane and the second factor is holomorphic in the lower half-plane. Of course, one can also isolate the zeros and poles so that the remaining factors are holomorphic and free of zeros. One then has a standard Wiener–Hopf factorization of the symbol S_l, which in this case is of modulus unity. For complex-valued functions such a factorization is trivial and can be done explicitly by quadrature.

When the potential in the Schrödinger equation is not central, on the other hand, matters are more complicated. If the particle described by the Schrödinger equation has an intrinsic spin then the direction dependence of the potential may be caused by its spin dependence so that the equation is form invariant under rotations and the total angular momentum is conserved. In that case the Schrödinger equation is still separable but with coupling between different orbital angular momenta. The S matrix for a given total angular momentum will then be a finite-dimensional square matrix, and so will the Jost function. In such a case, the Wiener–Hopf factorization is no longer trivial.[1,2]

In the most general case of a potential that depends on $x \in \mathbb{R}^3$ the Schrödinger equation cannot be separated and the S matrix is a function on $\mathbb{R}$ with values in the group $\mathcal{U}$ of unitary operators $L^2(S^2) \mapsto L^2(S^2)$, where S^2 is the unit sphere in $\mathbb{R}^3$. Physically, each point on S^2 stands for the asymptotic direction of the momentum of a particle. (If the Schrödinger equation is used for the description of waves other than quantum mechanical, then each point of S^2 stands for the direction of a wave vector.) In any case, the factorization of this operator-valued function remains an important tool in the study of the Schrödinger equation and particularly for the solution of the inverse-scattering problem. One kind of factorization leads to the generalization of the Jost function; another is a standard Wiener–Hopf factorization with respect to the real line. A third kind of factorization was introduced by Faddeev[3,4] (see also Ref. 5) in connection with another solution of the inverse scattering problem. We will not be concerned with that but will confine our attention to factorizations in which the factors are regarded as functions of the wave number (or the square root of the energy) and are continuous boundary values on the real line of analytic functions of that variable.

In Sec. II the two kinds of factorization of S that are of interest here are precisely defined; one is a standard Wiener–Hopf factorization with respect to the real line and the other is the Jost function factorization. Each leads to the definition of an index, one of which we call the Wiener–Hopf index and the other the Jost index. Some new results on the Jost factorization and, particularly, on the relation between the two factorizations are given; the most important one is Theorem 2.11. In Sec. III the Jost function factorization is implemented by the known technique of the generalized Marchenko equations and new results are contained in Theorem 3.1. Up to this point no assumption has been made about the admissibility of S as an S matrix of the Schrödinger equation. In Sec. IV this assumption is added and a third index, the Levinson index, is defined. Theorem 4.7 is the principal result of this section. In Sec. V the results of Secs. III and IV are applied to the inverse scattering problem and a new necessary and sufficient condition for the admissibility of a given S

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matrix is presented. Section VI contains all the proofs that are too long to be included in the earlier sections.

Notation: $\tilde{A}$ and $\overline{A}$ denote the operators whose integral kernels are, respectively, the transpose and the complex conjugate of that of A; $A^\dagger$ is the adjoint of A; nul A is the nullspace of A, ran A is its range, tr A is its trace, and $\mathbb{1}$ is the identity operator. We will usually denote operators by the same letters as their integral kernels. If f is a function on $\mathbb{R}$ then $f^\#(k) := f(-k)$; if g is a function on the unit sphere $\mathbb{S}^2$ in $\mathbb{R}^3$ then the operator Q is defined by $(Qg)(\theta) := g(-\theta)$; θ will denote both a point on $\mathbb{S}^2$ and the corresponding unit vector in $\mathbb{R}^3$.

II. FACTORIZATIONS DEFINED

Let us begin by defining a class of functions (sometimes called *symbols* in this context) in whose factorization we are interested.

Definition 2.1: $S\in\mathfrak{S}$ if and only if $S(k) = \mathbb{1} - (k/2\pi i)A(k)$, where $\mathbb{1}$ is the unit operator and the following six conditions are satisfied:

(i) The kernel $A(k,\theta,\theta')$ that defines the operator family $A(k)$, $k\in\mathbb{R}$, with values in the ring of bounded operators $L^2(\mathbb{S}^2)\mapsto L^2(\mathbb{S}^2)$, is a continuous, uniformly bounded, differentiable function $\mathbb{R}\times\mathbb{S}^2\times\mathbb{S}^2\mapsto\mathbb{C}$;

(ii) $QAQ = \tilde{A}$; this is called *reciprocity*;

(iii) $A(-k) = \overline{A(k)}$;

(iv) $S^\dagger S = SS^\dagger = \mathbb{1}$; *unitarity*;

(v) $\|S-\mathbb{1}\|\in L^2(\mathbb{R})$; $\|\cdot\|$ here is the operator norm;

(vi) the operators $\mathcal{G}$ and $\mathcal{G}^\#$ defined by (1), (2), and (3) in terms of A are compact.

We need the following functions:

$$\mathsf{G}(\alpha,\theta,\theta') := \frac{i}{(2\pi)^2}\int_{-\infty}^{\infty} dk\, kA(k,-\theta,\theta')e^{-ik\alpha}, \tag{1}$$

$$\mathcal{G}(\alpha,\theta;\beta,\theta') := \mathsf{G}(\alpha+\beta,\theta,\theta'), \quad \alpha,\beta\in\mathbb{R}_+,\ \theta,\theta'\in\mathbb{S}^2, \tag{2}$$

$$\mathcal{G}^\#(\alpha,\theta;\beta,\theta') := \mathsf{G}(-\alpha-\beta,\theta,\theta'), \quad \alpha,\beta\in\mathbb{R}_+,\ \theta,\theta'\in\mathbb{S}^2, \tag{3}$$

$$\mathcal{H}(\alpha,\theta;\beta,\theta') := \mathsf{G}(\alpha-\beta,\theta,\theta'), \quad \alpha,\beta\in\mathbb{R}_+,\ \theta,\theta'\in\mathbb{S}^2. \tag{4}$$

These integral kernels define the operators $\mathcal{G}$, $\mathcal{G}^\#$, $\mathcal{H}$; the first two are self-adjoint and the unitarity of S implies that $\|\mathcal{G}^2\|\leqslant 1$ and $\|\mathcal{G}^{\#2}\|\leqslant 1$, whereas $\mathcal{H}^\# = \mathcal{H}^\dagger$ (Ref. 5). Item (vi) and these operators will play a role in the implementation of the needed factorization, to be discussed later.

If S is admissible as an S matrix of the Schrödinger equation with a potential that is in a specified class, then $S\in\mathfrak{S}$. For example, the following class will do.

Definition 2.2: $\mathscr{V}_0 = \{V \mid V\in\mathbb{R}, \lim_{|x|\to\infty} V(x) = 0$, and $\exists a,C,\epsilon>0$, such that for all $x\in\mathbb{R}^3$, $|\nabla V(x)| < C(a+|x|)^{-4-\epsilon}\}$.

This class is smaller than it needs to be but it is easy to define. A larger class, called $\mathscr{W}$, which contains $\mathscr{V}_0$ and which also guarantees that $S\in\mathfrak{S}$, is defined in Ref. 5.

A standard left Wiener–Hopf factorization of S (also called *proper*)[6-9] with respect to the real line is a decomposition of the form

$$S = W_+ DW_-,$$

where

$$D = P_0 + \sum_{j\geqslant 1} P_j\left(\frac{k+i}{k-i}\right)^{\rho_j}. \tag{5}$$

The P_j, $j\geqslant 1$, are mutually orthogonal one-dimensional projections, $P_j = P_j^2$, $\operatorname{tr} P_j = 1$, $P_jP_i = 0$ if $i\neq j$, and $P_0 = \mathbb{1} - \Sigma_{j\geqslant 1}P_j$; $W_\pm$ is holomorphic and invertible everywhere in $\mathbb{C}^\pm$, $\lim_{|k|\to\infty}\|W_\pm - \mathbb{1}\| = 0$, and the *partial indices* ρ_j are nonzero integers. If $D = \mathbb{1}$ then the factorization is called *canonical* (or *regular*). Whereas the partial indices are uniquely determined by S, the factors $W_\pm$ and D are not. (However, if a canonical factorization exists, it is unique.) The sum of the partial indices is called the *total index* or the *sum index*. We shall call it the *Wiener–Hopf index* and denote it by

$$\operatorname{ind}_{\mathrm{WH}} S := \sum_j \rho_j.$$

It was proved by Aktosun and van der Mee[10] that if the potential underlying a given S is in a class that they specified ($V\in\mathscr{V}_0$ would do if zero is not an exceptional point of the Schrödinger equation) then S has a left standard factorization. They also showed that if $S = QS^{\#-1}Q$ (which is the case if $S\in\mathfrak{S}$) and S has a left standard factorization $S = W_+DW_-$ then it is always possible to choose the factorization in such a way that $W_- = QW_+^{\#-1}Q$, in other words,

$$S = QWQDW^{\#-1}. \tag{6}$$

It follows that in that case $DQ = QD$, because $D^\# = D^{-1}$. It is a characteristic of the standard factorization that the poles are in fixed positions at $\pm i$ and of a standard form.

The Jost function factorization, on the other hand, which is needed for the solution of the inverse scattering problem, is of a different kind. Here the factors are required to be meromorphic with *simple* poles at specified positions (on the imaginary axis) that are not standard, and moreover the residues are to be operators that have specified finite-dimensional ranges.[11] These data are collected in the following set.

Definition 2.3: The set $\mathscr{B}$ consists of all finite sets σ of p_σ pairs $\{\kappa_m,\mathscr{H}_m\}$ consisting of a positive number κ_m and a δ_m-dimensional subspace $\mathscr{H}_m$ of $L^2(\mathbb{S}^2)$ ($\delta_m < \infty$). The set $\{\delta_m\}$ will be denoted by $\mathbf{N}_\sigma$ and their sum by n_σ, $n_\sigma = \Sigma\delta_m$; the set $\{\kappa_m\}$ will be called $\mathbf{P}_\sigma$.

It is important for the inverse scattering problem that the set $\sigma\in\mathscr{B}$ that specifies all the bound-state data can be determined from the scattering amplitude.[5] However, for our purposes here that fact is of no significance.

We also need to define a class of relevant functions.

Definition 2.4: $\mathscr{M}^+$ is the set of all functions $\mathbb{R}\mapsto L^2(\mathbb{R})$ with values in the ring of bounded operators $[L^2(\mathbb{S}^2)\mapsto L^2(\mathbb{S}^2)]$ that are boundary values of analytic functions, meromorphic in $\mathbb{C}^+$, and whose operator norm approaches zero at infinity there. Similarly, $\mathscr{N}^+$ is the set of functions in $\mathscr{M}^+$ that are holomorphic in $\mathbb{C}^+$.

One then poses a Riemann–Hilbert problem with operator-valued solutions.

Problem $\mathscr{W}^1_\sigma(S)$: Let $S\in\mathfrak{S}$ and $\sigma\in\mathscr{B}$ be given. Find F such that

(i) $F-\mathbb{1}\in\mathscr{M}^+$, with simple poles at the points $i\kappa_m$,

$\kappa_m \in \mathbf{P}_\sigma$, and residues there whose ranges equal $\mathscr{H}_m$;

(ii) on $\mathbb{R}$, F satisfies the equation

$$F^\# = QS^\# FQ. \tag{7}$$

If the set σ is empty, we shall denote the corresponding problem by W_0^1, and if, in addition, (i) reads $F \in \mathscr{M}^+$, we denote it by W_0^0.

If this problem has a solution that is invertible, with an inverse that is holomorphic in $\mathbb{C}^+$, then this inverse is the *Jost function* and we have achieved a factorization of the form

$$S = QFQF^{\#-1}. \tag{8}$$

This is very similar to (6), except that the prescribed poles are in the factor function F itself and their form is more specifically given.

The factorization defined by W_σ^1 is not necessarily unique: For given S and σ the problem $W_\sigma^1(S)$ may have more than one solution; moreover, in general more than one set σ exists such that $W_\sigma^1(S)$ has a solution for a given S. The following lemma will be proved in Sec. VI.

Lemma 2.5: Suppose that the problem $W_\sigma^1(S)$ has a holomorphically invertible solution. Then for every choice of $\mathbf{P}_\mu$ with $p_\mu \leqslant n_\sigma$ there exist sets $\mu \in \mathscr{B}$ with $n_\mu = n_\sigma$ such that $W_\mu^1(S)$ also has a holomorphically invertible solution.

In other words, the pole positions in σ can be shifted at will without destroying the existence of a holomorphically invertible solution, and, as the proof shows, so can the ranges of the residues to a certain extent. The latter, however, cannot be changed completely freely.[12] The sum of the dimensions of the ranges of the residues, on the other hand, is fixed, as the following proposition asserts.

Proposition 2.6: Suppose that the problem $W_\sigma^1(S)$ has a holomorphically invertible solution. Then

(i) a necessary condition for another problem $W_\mu^1(S)$ to have a holomorphically invertible solution is that $n_\sigma = n_\mu$;

(ii) there exists another set $\mu \in \mathscr{B}$ with $\mathbf{P}_\mu$ and $n_\mu = n_\sigma + m$ (where m is a non-negative integer) arbitrarily given, such that $W_\mu^1(S)$ has a solution F whose inverse F^{-1} has m simple poles in $\mathbb{C}^+$.

Proof: The first part of this theorem combines Lemma 2.5 and the Index Theorem 2.6.8 of Ref. 5. To prove the second part we add and remove poles and zeros (i.e., poles of the inverse) just as we remove poles and add new ones in the proof of Lemma 2.5. ●

The second part of this theorem tells us that if we are willing to allow zeros in the solution, in the sense that its inverse has poles, then we can arbitrarily increase the number of poles in the solution sought. The first part of the theorem justifies defining a non-negative integer which we call the *Jost index*, by the following.

Suppose that $W_\sigma^1(S)$ has a holomorphically invertible solution F. Then

$$\text{ind}_J S := n_\sigma.$$

In other words, $\text{ind}_J S$ is the sum of the dimensions of the ranges of the residues of F at all its (simple) poles in $\mathbb{C}^+$.

The following lemma, which was first proved as Corollary 5.2 of Ref. 10, relates the *canonical* factorization of S to the problem $W_0^1(S)$. (Recall that if $S \in \mathfrak{S}$ then $S^{-1} = QS^\# Q$.)

Lemma 2.7: Suppose that $S^{-1} = QS^\# Q$. Then S has a left canonical factorization $S = W_+ W_-$ if and only if $W_0^1(S)$ has a solution F that is holomorphically invertible. We then have $F = QW_+ Q$, $W_- = QW_+^{\#-1} Q$, and F is the unique solution of $W_0^1(S)$.

A convenient tool in the study of the more general case with poles is the reduction method.[13,5] It utilizes the rational function

$$\Pi_\sigma := \left(\mathbb{1} - B_1 + B_1 \frac{k + i\kappa_1}{k - i\kappa_1}\right) \times \left(\mathbb{1} - B_2 + B_2 \frac{k + i\kappa_2}{k - i\kappa_2}\right) \cdots . \tag{9}$$

Here, the B_j are self-adjoint projections that are successively constructed so that the function $F^{\text{red}} := \Pi_\sigma^{-1} F$ is free of poles. They are uniquely determined by the spaces $\mathscr{H}_m$ in σ. The solvability of $W_\sigma^1(S)$ may thus be reduced to the existence of a canonical factorization of the reduced S matrix.

Lemma 2.8: If $W_\sigma^1(S)$ has a holomorphically invertible solution F then $S^{\text{red}} := Q\Pi_\sigma^{-1} QS\Pi_\sigma^\#$ has a left canonical factorization; conversely, if S^{red} has a left canonical factorization, then $W_\sigma^1(S)$ has a unique solution F and the inverse F^{-1} is holomorphic in $\mathbb{C}^+$. Here, Π_σ is the factor of the form (9) appropriate for W_σ^1.

Proof: Suppose that S^{red} has a left canonical factorization. Then by Lemma 2.7 $W_0^1(S^{\text{red}})$ has a unique solution F^{red}, $F := \Pi_\sigma F^{\text{red}}$ solves $W_\sigma^1(S)$ uniquely, and $(F^{-1} - \mathbb{1}) \in \mathscr{N}^+$. Conversely, if $W_\sigma^1(S)$ has a holomorphically invertible solution F then $F^{\text{red}} := \Pi_\sigma^{-1} F$ solves $W_0^1(S^{\text{red}})$ and is holomorphically invertible. Hence, by Lemma 2.7 S^{red} posesses a left canonical factorization. ●

If a left standard factorization exists, however, the most powerful procedure is to reduce the solvability of $W_\sigma^1(S)$ to a similar problem for the diagonal factor, which is a rational function. We prove the following in Sec. VI.

Lemma 2.9: Suppose that $S = QS^{\#-1} Q$ has the left standard factorization $S = W_+ DQW_+^{\#-1} Q$. Then the following holds.

If $W_\sigma^1(S)$ has a unique solution then there exists a set $\sigma' \in \mathscr{B}$ with $\mathbf{P}_{\sigma'} = \mathbf{P}_\sigma$ and $\mathbf{N}_{\sigma'} = \mathbf{N}_\sigma$ such that $W_{\sigma'}^1(D)$ has a unique solution, and vice versa.

If $W_\sigma^1(D)$ has a unique solution then $\exists \sigma' \in \mathscr{B}$ with $\mathbf{P}_{\sigma'} = \mathbf{P}_\sigma$ and $\mathbf{N}_{\sigma'} = \mathbf{N}_\sigma$ such that $W_{\sigma'}^1(S)$ has a unique solution.

The same holds if "unique" is everywhere replaced by "holomorphically invertible."

The problem $W_\sigma^1(D)$ for the rational function D, on the other hand, is solved by the following result.

Lemma 2.10: Suppose that

$$D = P_0 + \sum_{j \geqslant 1} P_j \left(\frac{k+i}{k-i}\right)^{\rho_j} \neq \mathbb{1},$$

$P_j = P_j^2$, $\text{tr}\, P_j = 1$, $j \geqslant 1$, $P_0 + \Sigma_{j>1} P_j = \mathbb{1}$, $P_j P_i = 0$ if $i \neq j$, all the ρ_j are nonzero integers, and $QD = DQ$. A necessary condition for the problem $W_\sigma^1(D)$ to have a holomorphically invertible solution is that (1) each ρ_j is even and positive,

and (2) $n_\sigma = \frac{1}{2}\Sigma_j \rho_j$. Conversely, if each ρ_j is even and positive, then there exists a set $\sigma \in \mathscr{B}$ with $n_\sigma = \frac{1}{2}\Sigma_j \rho_j$ such that the problem $W^1_\sigma(D)$ has a holomorphically invertible solution.

This, too, is proved in Sec. VI.

The combination of Lemmas 2.9 and 2.10 allows us to conclude the following theorem.

Theorem 2.11: Suppose that $S = QS^{\#-1}Q$ has a left standard factorization. Then the following two conditions are necessary for the problem $W^1_\sigma(S)$ to have a holomorphically invertible solution:

(1) either S has no left partial indices, or each left partial index of S is even and positive;

(2) $n_\sigma = \frac{1}{2}\,\mathrm{ind}_{\mathrm{WH}}\, S$.

Conversely, if (1) holds, then there exists a set $\sigma \in \mathscr{B}$ with $n_\sigma = \frac{1}{2}\,\mathrm{ind}_{\mathrm{WH}}\, S$ and arbitrarily prescribed $\mathbf{P}_\sigma$ such that the problem $W^1_\sigma(S)$ has a holomorphically invertible solution.

It should be noted that the set σ for which $W^1_\sigma(S)$ has a holomorphically invertible solution is not entirely freely at our disposal once a left standard factorization is given. That is why these results always refer to the *existence* of a set $\sigma \in \mathscr{B}$ such that W^1_σ has a holomorphically invertible solution. They do not assert that such a solution exists for *all* $\sigma \in \mathscr{B}$ with $n_\sigma = \frac{1}{2}\,\mathrm{ind}_{\mathrm{WH}}\, S$.

III. IMPLEMENTING A FACTORIZATION

The solution of the problem $W^1_\sigma(S)$ is implemented by Fourier transformation as follows.[5] Define n_σ functions $\mathbb{R}_+ \times \mathbb{S}^2 \mapsto \mathbb{C}$,

$$y^b_m(\alpha,\theta) = Y^b_{\kappa_m}(-\theta)e^{-\alpha\kappa_m}, \tag{10}$$

where the functions $Y^b_{\kappa_m}$, $b = 1,\ldots,\delta_m$, span the space $\mathscr{H}_m$ and $\kappa_m \in \mathbf{P}_\sigma$. Let the functions $z^{[n]}_\pm$ span the null spaces of $(\mathbb{1} \pm \mathscr{G}^\#)$, respectively. Then define the matrices $s^\pm$ with the elements

$$s^\pm_{n,mb} = \langle z^{[n]}_\pm, y^b_m \rangle_+, \tag{11}$$

and the column matrices $c_\pm(\theta)$ with the elements

$$c^{[n]}_\pm(\theta) := \langle z^{[n]}_\pm, \mathsf{G}^\#_\pm \rangle_+(\theta). \tag{12}$$

Here, $\langle \cdot,\cdot \rangle_+$ is the inner product on $L^2(\mathbb{R}_+ \times \mathbb{S}^2)$ and $\mathsf{G}^\#(\alpha,\theta',\theta) := \mathsf{G}(-\alpha,\theta',\theta)$ is to be regarded as a family of vectors in $L^2(\mathbb{R}_+ \times \mathbb{S}^2)$ parametrized by $\theta \in \mathbb{S}^2$; $\mathsf{G}_\pm := \mathsf{G}\frac{1}{2}(\mathbb{1} \pm \mathsf{Q})$.

The generalized Marchenko equations then are the following two Fredholm equations of the second kind on $\mathbb{R}_+ \times \mathbb{S}^2$:

$$(\mathbb{1} \mp \mathscr{G})\Gamma_\pm = \pm \mathsf{G}_\pm \pm (\mathsf{Q} + \mathscr{H})\mathscr{Y}_\pm, \tag{13}$$

where $\Gamma = \Gamma_+ + \Gamma_-$ is related to the sought solution $F(k)$ of $W^1_\sigma(S)$ by

$$\Gamma(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\,[F(k) - \mathbb{1}]e^{-ik\alpha}, \tag{14}$$

$$\mathscr{Y}_\pm(\alpha,\theta,\theta') := \sum_{m,b} y^b_m(\alpha,\theta)\rho^{mb}_\pm(\theta'),$$

and the functions $\rho^{mb}_\pm$ are to be determined by the set of linear algebraic equations

$$c^{[n]}_\pm(\theta) = 2\sum_{m,b} s^\pm_{n,mb}\rho^{mb}_\pm(\theta). \tag{15}$$

Remark: Clearly, the unique solvability of Eqs. (15) depends on the invertibility of the matrices $s^\pm$. Let us call $\mathfrak{Y}$ the linear span of the functions y^b_m defined in (10). Then we may state the existence of inverses of the matrices $s^\pm$ geometrically: *The matrices* $s^\pm$ *are invertible if and only* if $\mathfrak{Y}_1 \cup \mathrm{nul}(\mathbb{1} \pm \mathscr{G}^\#) = \{0\}$, *respectively*. Since $\mathscr{G}^\#$ is self-adjoint and hence $\mathrm{nul}(\mathbb{1} \pm \mathscr{G}^\#)_\perp = \mathrm{ran}(\mathbb{1} \pm \mathscr{G}^\#)$, this may also be stated in the equivalent form: *The matrices* $s^\pm$ *are invertible if and only if* $\mathfrak{Y} \cup \mathrm{ran}(\mathbb{1} \pm \mathscr{G}^\#) = \{0\}$, *respectively*.

A part of the following theorem was proved in Ref. 5 and the rest of it will be proved in Sec. VI.

Theorem 3.1: The following three statements are equivalent:

(a) The problem $W^1_\sigma(S)$ has a unique solution F.

(b) The problem $W^1_\sigma(S)$ has a solution F that is holomorphically invertible, i.e., $(F^{-1} - \mathbb{1}) \in \mathscr{N}^+$.

(c) The following three conditions hold:

(i) the operator $\mathscr{G}^2$ does not have the eigenvalue 1,

(ii) $\dim \mathrm{nul}(\mathbb{1} + \mathscr{G}^\#) = \dim \mathrm{nul}(\mathbb{1} - \mathscr{G}^\#) = n_\sigma$,

(iii) the matrices $s^\pm$ of (11) are invertible.

If one of the conditions (a)–(c) is satisfied then the solution F is obtained from the solutions of (13) by

$$F(k,\theta,\theta') = \mathbb{1} + \int_0^\infty d\alpha\, e^{ik\alpha}\Gamma(\alpha,\theta,\theta') + \sum_{m,b} \frac{Y^b_{\kappa_m}(\theta)\rho^{mb}(\theta')}{i(k - i\kappa_m)},$$

where $\Gamma = \Gamma_+ + \Gamma_-$ and $\rho^{mb} := \rho^{mb}_+ + \rho^{mb}_-$.

Note that if S is given, then $\mathscr{G}$ and $\mathscr{G}^\#$ are given, and hence, so are the null spaces of $\mathbb{1} \pm \mathscr{G}^\#$. Therefore, the number $n_\sigma = \mathrm{ind}_J\, S$ of the problem $W^1_\sigma(S)$ that has a unique solution, if it exists, can be determined directly from S. The question is, does such a problem $W^1_\sigma(S)$ always exist if $\mathscr{G}^2$ does not have the eigenvalue 1? First, we have the following result, which will be proved in Sec. VI.

Lemma 3.2: Given S and $\mathbf{P}_\sigma$ in a set $\sigma \in \mathscr{B}$ with $n_\sigma = \dim \mathrm{nul}(\mathbb{1} + \mathscr{G}^\#) = \dim \mathrm{nul}(\mathbb{1} - \mathscr{G}^\#) \geqslant p_\sigma$, there always exist n_σ functions $Y^b_{\kappa_m}$ so that the matrices $s^\pm$ defined in (11) are invertible.

As a consequence, the following proposition holds.

Proposition 3.3: Suppose that $S \in \mathfrak{S}$ is such that the operator $\mathscr{G}^2$ does not have the eigenvalue 1 and $\dim \mathrm{nul}(\mathbb{1} + \mathscr{G}^\#) = \dim \mathrm{nul}(\mathbb{1} - \mathscr{G}^\#) := N$. Then there exists a set $\sigma \in \mathscr{B}$ with $n_\sigma = N$ such that the problem $W^1_\sigma(S)$ has a unique solution. Moreover, the set $\mathbf{P}_\sigma$ can be chosen at will, so long as $p_\sigma \leqslant n_\sigma$.

IV. ADMISSIBLE S MATRICES

We have, so far, made no assumptions concerning the admissibility of the given symbol S, i.e., we have not assumed that it is a Schrödinger S matrix for which there exists an underlying potential. If a potential exists, for example in $\mathscr{V}_0$, and it causes N bound states of negative energy (let us assume that zero is not an exceptional point) then this num-

ber can be recognized from S by means of the generalized Levinson theorem. This leads to the definition of a third kind of index in terms of the total phase change of the Fredholm determinant of S. Since that Fredholm determinant generally does not approach unity as $k\to\infty$ even though $\|S-\mathbb{1}\|$ approaches naught, we have to proceed with caution.

Definition 4.1: The function $S:\mathbb{R}\to\mathscr{U}$ is in $\mathbb{U}$ if and only if it has the following properties:

(i) S is continuous; (ii) $S^{\#}=\bar{S}$; (iii) $\lim_{k\to 0}\|S(k)-\mathbb{1}\|=0$; (iv) for each $k\in\mathbb{R}$ the Fredholm determinant $\det S$ exists; (v) $\exists c_1, c_2$ such that as $k\to\infty$

$$\delta(k)=c_1k+c_2+o(1),$$

where $\delta(k)=\frac{1}{2}\arg\det S(k)$ is defined to be continuous,

$$\det S(k)=e^{2i\delta(k)}.$$

The operator $S-\mathbb{1}$ being compact if $S\in\mathbb{S}$, the unitary S has a point spectrum only. Its eigenvalues $e^{2i\eta_n}$ define the eigenphase shifts η_n. Since $\lim_{|k|\to\infty}\|S-\mathbb{1}\|=0$, each eigenphase shift can be defined so as to approach naught as $|k|\to\infty$. The phase δ defined above is related to the eigenphase shifts by $\delta(k)=\Sigma\eta_n(k)$, but the convergence of the series is not uniform in k: Even though $\lim_{k\to\infty}\eta_n(k)=0$ for each n, their sum grows linearly as $k\to\infty$. If the potential $V\in\mathscr{V}_0$ then $S\in\mathbb{U}$, c_2 is an integral multiple of π, and it is always permissible to choose $c_2=0$ (Ref. 5), which we shall do. Item (iii) in the above definition implies that there are no half-bound states. We now define the *Levinson index* of S by

$$\mathrm{ind}_L\ S:=(1/\pi)\delta(0).$$

A three-dimensional generalization of Levinson's theorem[13] can then be stated in the following form.

Generalized Levinson's theorem: If S is the S matrix of a potential $V\in\mathscr{W}$ that produces N bound states (counting their multiplicities) and there is no half-bound state, then $\mathrm{ind}_L\ S=N$.

Thus if S is admissible and there is no half-bound state, then $\mathrm{ind}_L\ S$ is a non-negative integer. It is related to the Wiener–Hopf index by the following result, which will be proved in Sec. VI.

Lemma 4.2: If $S=QS^{\#-1}Q$, $S\in\mathbb{U}$, and it has a left standard factorization then $\mathrm{ind}_L\ S=\frac{1}{2}\mathrm{ind}_{WH}\ S$.

Now, if we are given an S matrix that is admissible, with a potential that leads to N bound states, then we seek a factorization with N poles; in other words, we pose $W^1_\sigma(S)$ with $n_\sigma=N$. By Theorem 3.1 we then need $N=\dim\mathrm{nul}(\mathbb{1}+\mathscr{G}^{\#})=\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{\#})$. The following lemma assures that this requirement is, in fact, satisfied; it will be proved in Sec. VI.

Lemma 4.3: If S is admissible and the underlying potential causes N bound states of negative energy (counting their multiplicities) then $\dim\mathrm{nul}(\mathbb{1}+\mathscr{G}^{\#})=\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{\#})=N$.

The following lemma will also be proved in Sec. VI.

Lemma 4.4: If S is admissible then the matrices $s^{\pm}$ defined in (11) are invertible.

Let us define

$$S_x(k,\theta,\theta'):=S(k,\theta,\theta')e^{ikx\cdot(\theta-\theta')},\quad x\in\mathbb{R}^3,\qquad(16)$$

which is the S matrix of a potential shifted by x; $A_x=(2\pi i/k)(\mathbb{1}-S_x)$ is the corresponding scattering amplitude. The number of bound states produced by a potential is invariant under such a shift. Lemma 4.3 therefore has the following corollary.

Corollary 4.5: Suppose that $\mathscr{G}$ corresponds to the S matrix S_x defined in (16), where S is admissible, and thus $\mathscr{G}^{\#}$ depends on x. Then the dimensions of the null spaces of $(\mathbb{1}\pm\mathscr{G}^{\#})$ do not depend on x.

Finally, we have an important result whose proof is based on a known theorem for the standard Wiener–Hopf factorization, as well as on Lemmas 4.2 and 4.3.

Lemma 4.6: If S is admissible with a potential $V\in\mathscr{W}$ and no exceptional point at $k=0$, then $\|\mathscr{G}\|<1$.

Proof: Since the unitarity if the S matrix implies that $\|\mathscr{G}\|\leqslant 1$ and since $\mathscr{G}$ is compact if $S\in\mathbb{S}$, the theorem follows if we prove that $\mathscr{G}^2$ does not have the eigenvalue 1. The following formula follows directly from Theorem 1.1 of Ref. 9, p. 165, and formulas (2.26) and (2.28) of Ref. 5.

$$\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{\#2})-\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{2})=\mathrm{ind}_{WH}\ S.$$

Using Lemma 4.3 we get

$$\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{2})=\dim\mathrm{nul}(\mathbb{1}-\mathscr{G}^{\#2})-\mathrm{ind}_{WH}\ S=2N-\mathrm{ind}_{WH}\ S,$$

where N is the number of bound states (counting their multiplicities). Therefore, the desired result follows from the generalized Levinson theorem together with Lemma 4.2. ●

The following theorem now is a direct consequence of Lemmas 4.3, 4.4, 4.6, and Theorem 3.1.

Theorem 4.7: If S is admissible as an S matrix of the Schrödinger equation with a potential in $\mathscr{W}$ that causes n_σ bound states (counting their multiplicities δ_m) with data collected in $\sigma\in\mathscr{B}$ (in the sense that $\mathbf{P}_\sigma$ consist of the κ_m if the eigenvalues are $-\kappa_m^2$ and the $\mathscr{H}_m$ are the spans of the corresponding characters), then $W^1_\sigma(S)$ has a unique (and hence holomorphically invertible) solution.

V. APPLICATION TO THE INVERSE SCATTERING PROBLEM

The results we have obtained answer some important questions left open in our previous studies of the inverse scattering problem for the Schrödinger equation in $\mathbb{R}^3$. In particular, this includes the existence of the Jost function (and thus of the "regular solution"[5]) and the unique solvability of the generalized Marchenko equation. The vector version of the latter, which is the equation needed for the solution of the inverse-scattering problem by the generalized Marchenko method, is obtained by letting Eqs. (13) act on the vector $\hat{1}$ which is defined as the constant function identically equal to 1, and setting $\eta:=\Gamma_+\hat{1}$ and $\mathbf{g}:=\mathbf{G}_+\hat{1}$. Lemmas 4.6, 4.3, and 4.4, together with Theorem 2.4.7 of Ref. 5 then imply the following necessary and sufficient conditions for the existence of an underlying potential.

Theorem 5.1: Let S be the S matrix of the Schrödinger equation with a given potential in $\mathscr{W}$ that has the following bound-state properties:

(*) it causes N bound states (counting their multiplicities) of negative energies $-\kappa_m^2$ with eigenfunctions $p^{mb}(x)$

and characters $Y^b_{\kappa_m}(\theta)$, and $k=0$ is not an exceptional point.

Define S_x as in (16) and the operators $\mathscr{G}$ and $\mathscr{G}^\#$ by (1), (2), and (3) in terms of $A_x=(2\pi i/k)(\mathbb{1}-S_x)$ (so that they depend parametrically on $x\in\mathbb{R}^3$). Then the following conditions hold:

(i) $S\in\mathfrak{S}$;

(ii) $\mathrm{ind}_L S=N$;

(iii) S satisfies item (viii) of Definition 1.5.15 on p. 28 of Ref. 5 (forward analyticity);

(iv) if $N=0$ then $\mathscr{G}^\#$ does not have the eigenvalues ± 1; if $N>0$ then $\mathscr{G}^\#$ has the eigenvalues ± 1 and each of the two corresponding eigenspaces is N dimensional;

(v) the generalized Marchenko equation has a unique solution:

$$\eta=\mathbf{g}+(Q+\mathscr{H})\mathfrak{P}+\mathscr{G}\eta, \tag{17}$$

where $\mathfrak{P}$ is given by

$$\mathfrak{P}(\alpha,\theta):=\sum_{m,b} y^b_m(\alpha,\theta)p^{mb}$$

and the p^{mb} are the unique solution of the set of linear algebraic equations

$$c^{[n]}=2\sum_{m,b} s^+_{n,mb}p^{mb}; \tag{18}$$

here, $s^+_{n,mb}$ are given by (11), the $z^{[n]}_+$ form a basis in the eigenspace of $\mathscr{G}^\#$ at the eigenvalue -1, the functions y^b_m are defined by (10), and the numbers $c^{[n]}$ are defined by (12); in other words, the operator $\mathscr{G}$ does not have the eigenvalue 1 (so that $\|\mathscr{G}\|<1$) and the matrix s^+ is invertible; moreover, this solution is miraculous (i.e., the right-hand side of (19) is independent of θ);

(vi) the Jost function with all the required properties exists.

Conversely, let S be given and let S_x be defined as before. If S_x satisfies conditions (i)–(v) for almost all $x\in\mathbb{R}^3$, then the function ψ defined by

$$\psi(k,\theta,x)=e^{ik\theta\cdot x}+\int_{\theta\cdot x}^{\infty} e^{ik\alpha}\eta(\alpha-\theta\cdot x,\theta,x)+\sum_{m,b}\frac{p^{mb}(x)\,Y^b_{\kappa_m}(-\theta)}{i(k-i\kappa_m)}e^{i(k-i\kappa_m)\theta\cdot x},$$

in terms of the unique solution η of (17) and p^{mb} of (18) satisfies the Schrödinger equation with the potential

$$V(x)=-2\theta\cdot\nabla\Big[\eta(\alpha=0+,\theta,x)-\sum_{m,b} y^b_m(-\theta\cdot x,\theta,x)p^{mb}(x)\Big], \tag{19}$$

which has the bound-state properties (*). Moreover, ψ satisfies the scattering boundary condition and the function $A=(2\pi i/k)(\mathbb{1}-S)$ is the corresponding scattering amplitude.

Except for the lack of specification of the class in which the potential lies, this theorem constitutes a *necessary and sufficient condition* for, and thus a *characterization* of, the admissibility of a given scattering amplitude or S matrix.

VI. PROOFS

Proof of Lemma 2.5: Assume that F solves $W^1_\sigma(S)$, in which one of the poles is stipulated to be at $k=i\kappa$, and let the residue of F there be R. Define $F_\pm:=F(\mathbb{1}\pm Q)/2$, so that $F^\#_\pm=\pm QS^\#F_\pm$, and $F=F_+ +F_-$; define also $F'_\pm:=F_\pm\Pi_\pm$,

$$\Pi_\pm:=\mathbb{1}+C_\pm[(\kappa^2-\nu^2)/(k^2+\nu^2)].$$

Let $R_\pm$ be the residue of $F_\pm$ at $k=i\kappa$ and take $C_\pm$ so that $R_\pm(\mathbb{1}-C_\pm)=0$. Then $F'_\pm$ are holomorphic at $k=i\kappa$. Since $R_\pm=R(\mathbb{1}\pm Q)/2$, we define $C_\pm=C^2_\pm$ to be projections (but not necessarily self-adjoint) whose null spaces equal those of $R_\pm$, and so that $C_\pm=(\mathbb{1}\pm Q)C_\pm/2=C_\pm(\mathbb{1}\pm Q)/2$, which is always possible. This implies that $C_+C_-=C_-C_+=0$ and $C:=C_++C_-$ is also a projection. We then define $F':=F'_++F'_-=F\Pi$, where

$$\Pi=\mathbb{1}+C[(\kappa^2-\nu^2)/(k^2+\nu^2)]$$

and find

$$F'^\#=F'^\#_+ +F'^\#_-=F^\#_+\Pi_+ +F^\#_-\Pi_-$$
$$=QS^\#(F_+\Pi_+Q-F_-\Pi_-Q)Q,$$

and one easily sees that $F_+\Pi_+Q-F_-\Pi_-Q=F'$. Therefore, F' satisfies (7).

The functions $F'_\pm$ have poles at $k=i\nu$ and their residues there are $R'_\pm=F_\pm(i\nu)C_\pm$. Thus F' has a pole there with residue

$$R'=R'_+ +R'_-=F_+(i\nu)C_+ +F_-(i\nu)C_-$$
$$=F(i\nu)[(\mathbb{1}+Q)C_+/2+(\mathbb{1}-Q)C_-/2]=F(i\nu)C.$$

Therefore, since $F(i\nu)$ is invertible, the dimension of the range of R' equals that of the range of C. Note that if F is holomorphically invertible, then clearly so is F'.

Since $\mathrm{nul}\,R=\mathrm{ran}(\mathbb{1}-C)=\mathrm{nul}\,C$ and C is a projection, $\mathrm{nul}\,R\cap\mathrm{ran}\,C=\{0\}$. It follows that $R=RC$ implies that the range of C has the same dimension as the range of R. Therefore, $\dim\mathrm{ran}\,R=\dim\mathrm{ran}\,C=\dim\mathrm{ran}\,R'$. Thus we conclude that F' is a solution of $W^1_\mu(S)$ in which one of the poles has been shifted to a new position, but the dimension of the range of the new residue is the same as that of the old. The range of the residue at the new pole can be almost arbitrarily assigned (except for its dimension) by proper choice of the range of $C_\pm$ since $F(i\nu)$ has an inverse. There is, however, one restriction: The range of $C_\pm$ must not be a subspace of its null space. This puts a restriction on the range of the residue R', the precise nature of which is unclear but of no consequence here.

Suppose, on the other hand, that we choose $\mathrm{nul}\,C=\mathrm{ran}(\mathbb{1}-C)\supset\mathrm{nul}\,R$ with $m:=\dim\mathrm{ran}\,C<\dim\mathrm{ran}\,R$. Then F still has a pole at $k=i\kappa$ with a residue $R(\mathbb{1}-C)$ such that $\dim\mathrm{ran}\,R(\mathbb{1}-C)=\dim\mathrm{ran}\,R-m$ and it also has a simple pole at $k=i\nu$ with residue $F(i\nu)C$ such that $\dim\mathrm{ran}\,F(i\nu)C=m$. Hence the sum of the dimensions of the ranges of the residues is unchanged.

If we choose $\mathrm{ran}(\mathbb{1}-C)\subset\mathrm{nul}\,R$ with $\dim\mathrm{ran}\,C>\dim$

ran R then F^{-1} will have a pole at $k = i\kappa$, which we do not want.

So we now know how to reduce the dimension of the range of the residue at one pole and to produce a new pole elsewhere, with no change in the sum of the dimensions of the ranges. (One may thus split off all poles so that they have residues with one-dimensional ranges.) How do we *increase* the dimension of the range of a residue?

Suppose that F has a simple pole at $k = i\nu$, so that

$$F = R\,[1/(k - i\nu)] + A + \cdots$$

and F^{-1} is holomorphic there. Suppose further that F has a simple pole at $k = i\kappa$ with residue R_0, whose range may be assumed to be one-dimensional. In order to remove the pole at $i\kappa$ and increase the range of the residue at $i\nu$ we form

$$F' := F(\mathbb{1} + C\,[(\kappa^2 - \nu^2)/(k^2 + \nu^2)])$$

with the projection C chosen so that $R_0(\mathbb{1} - C) = 0$ with $\dim \operatorname{ran} C = \dim \operatorname{ran} R_0$ (see the above argument) so as to remove the pole at $i\kappa$. If C is chosen so that $RC = 0$ then F' has a simple pole at $k = i\nu$ with the residue

$$R' = R + AC\,[(\kappa^2 - \nu^2)/2i\nu].$$

The fact that F^{-1} is holomorphic at $i\nu$ implies that $\exists D$, E such that

$$RE + AD = ER + DA = \mathbb{1},$$

which, in turn, implies that $\operatorname{nul} R \cap \operatorname{nul} A = \{0\}$ and the ranges of A and R decompose $L^2(\mathbb{S}^2)$. Therefore, $\dim \operatorname{ran} AC = \dim \operatorname{ran} C = \dim \operatorname{ran} R_0$ and $\dim \operatorname{ran} R' = \dim \operatorname{ran} R + \dim \operatorname{ran} AC = \dim \operatorname{ran} R + \dim \operatorname{ran} R_0$. Thus the sum of the dimensions of the ranges of the residues is preserved.

Finally, we may change the range of the residue of any pole without changing its position and dimension by shifting it first to a new position and then back. In this manner we may change the positions and ranges of the residues of all poles of a solution of $W^1_\sigma(S)$ so as to become a solution of $W^1_\mu(S)$, so long as $n_\sigma = n_\mu$ and the spaces $\mathscr{H}_m$ are properly chosen. ●

Proof of Lemma 2.9: Suppose that $W^1_\sigma(D)$ has the unique solution $f = \Pi' f'$, where $f' - \mathbb{1} \in \mathscr{N}^+$ (see Definition 2.4) and Π' has the structure (9) appropriate to W^1_σ. It then follows that $F := QW_+\,\Pi' f' Q$ satisfies $F^\# = QS^\# FQ$. There exists a function Π of the same structure as (9), with poles in the same positions and with projections on spaces of the same dimensions as those of Π', such that $W_+\,\Pi' = \Pi W'_+$. Therefore, F uniquely solves the problem $W^1_{\sigma'}(S)$, where the set σ' consists of the same pole positions as σ and the dimensions of the corresponding spaces $\mathscr{H}_m$ are the same. Since both D and Π' are meromorphic functions with finite numbers of poles and residues of finite-dimensional ranges, they are equivalent to finite-dimensional matrices, and so is f'; hence it is invertible and $f'^{-1} - \mathbb{1}$ is in $\mathscr{M}^+$; by Lemma 2.6.5 of Ref. 5, therefore, $f'^{-1} - \mathbb{1}$ is in $\mathscr{N}^+$ and so is F.

Conversely, suppose that F uniquely solves the problem $W^1_\sigma(S)$. We then reverse all the steps of the above argument and conclude that $W^1_{\sigma'}(D)$ must have a unique solution f. Again this solution is rational and "like a matrix," and hence invertible with $f^{-1} - \mathbb{1}$ in $\mathscr{N}^+$. The second part of the proposition is proved similarly. ●

Proof of Lemma 2.10: Suppose that the problem $W^1_\sigma(D)$ has a holomorphically invertible solution F, so that

$$F^\# = QD^\# FQ$$

with the appropriate analyticity and asymptotic properties. Multiplying the equation on the left by P_j and on the right by P_l leads to

$$P_j F^\# P_l = ((k - i)/(k + i))^\rho P_j F P_l,$$

since $QD = DQ$ implies that the one-dimensional projections $P_j, j \geqslant 1$, are such that $QP_j = P_j$. The requirement that $\lim_{|k|\to\infty} \|F - \mathbb{1}\| = 0$ leads to $P_j F P_l = 0$ for $l \neq j$, since the homogeneous Riemann–Hilbert problem defined by that equation has only the trivial solution. So we have $F = P_0 + \Sigma_j P_j f_j$, where each f_j solves the simple scalar Riemann–Hilbert problem

$$f^\# = ((k - i)/(k + i))^\rho f,$$

in which f is to have simple poles and no zeros in $\mathbb{C}^+$. (Zeros would produce poles in F^{-1}.) This problem has no solution unless ρ is a positive even integer. (For $\rho = 0$ the solution is $f = 1$, and that can be taken to be part of P_0.) If $\rho = 2m$ then a solution without zeros in $\mathbb{C}^+$ must have m poles and it is of the form

$$f = (k + i)^{2m}/(k^2 + \kappa_1^2)\cdots(k^2 + \kappa_m^2).$$

Therefore, we may conclude that all the ρ_j must be even, $\rho_j = 2m_j$, and the holomorphically invertible function F must be

$$F = P_0 + \sum_j P_j \frac{(k + i)^{2m_j}}{(k^2 + \kappa_1^2)\cdots(k^2 + \kappa_{m_j}^2)}. \tag{20}$$

It is easily seen that this F is such that

$$\sum_j \dim \operatorname{ran} \operatorname{Res}_{\kappa_j} = n_\sigma = \operatorname{ind}_J D = \sum_j m_j = \frac{1}{2} \operatorname{ind}_{WH} D.$$

Conversely, if each ρ_j is even then the function F given by (20) satisfies the equation $F^\# = QD^\# FQ$, is holomorphically invertible, and furthermore the sum of the dimensions of the ranges of the residues at its simple poles equals $\frac{1}{2}\Sigma_j \rho_j$. ●

Proof of Theorem 3.1: Most of this theorem coincides with Theorem 2.6.15 in Ref. 5. Item (b), however, is new. For the proof of this part we need the following two lemmas.

Lemma 6.1: If $W^1_\sigma(S)$ has a unique solution then $W^1_0(S^\#)$ has a solution.

Lemma 6.2: If $W^1_\sigma(S)$ and $W^1_\sigma(S^\#)$ have solutions F_1 and F_2, respectively, then $(F_1^{-1} - \mathbb{1}) \in \mathscr{M}^+$ and $(F_2^{-1} - \mathbb{1}) \in \mathscr{M}^+$.

Assume that S has property (a), i.e., that $W^1_\sigma(S)$ has a unique solution F_1. Then by Lemma 6.1 $W^1_0(S^\#)$ has a solution F_2, and hence by Lemma 6.2 $(F_1^{-1} - \mathbb{1}) \in \mathscr{M}^+$. By item (v) of Lemma 2.6.5 of Ref. 5 this implies that $(F_1^{-1} - \mathbb{1}) \in \mathscr{N}^+$. Thus (a) implies (b). The converse, namely the statement that if $W^1_\sigma(S)$ has a holomorphically invertible solution then its solution is unique, follows directly from Lemma 2.8.

There is, in addition, a gap in the proof of Theorem

2.6.15 in Ref. 5 [which is Theorem 3.1 without statement (b)]. Suppose that conditions (i) and (iii) of statement (c) are satisfied, but one of the elements of $\rho_\pm(\theta)$ vanishes for all θ. Then the sum of the dimensions of the range of a pole of the solution F of $W^1_\sigma(S)$ is lower than the dimension of the null space of $\mathbb{1}+\mathscr{G}^\#$, contrary to (ii). Since $\rho_\pm(\theta)=\frac{1}{2}s^{\pm-1}c_\pm(\theta)$, $\rho^n_\pm(\theta)\equiv 0$ implies that there exists a constant vector a such that $ac_\pm(\theta)\equiv 0$ for either $+$ or $-$ (or both). By definition (12), in turn, this would mean that there exists a vector $z_+\in\mathrm{nul}(\mathbb{1}+\mathscr{G}^\#)$ [or $z_-\in\mathrm{nul}(\mathbb{1}-\mathscr{G}^\#)$] such that $\langle z_+,\mathsf{G}^\#_+\rangle_+\equiv 0$ for all θ (or $\langle z_-,\mathsf{G}^\#_-\rangle_+\equiv 0$ for all θ). It follows from Lemma 2.6.10 of Ref. 5 that $\langle z_\pm,\mathsf{G}^\#_\mp\rangle_+(\theta)\equiv 0$ for every $z_+\in\mathrm{nul}(\mathbb{1}+\mathscr{G}^\#)$ and for every $z_-\in\mathrm{nul}(\mathbb{1}-\mathscr{G}^\#)$. Hence, the vanishing of one element of $\rho_\pm$ for all θ would imply that $\langle z_\pm,\mathsf{G}^\#\rangle_+(\theta)\equiv 0$ for some z_+ or z_-. The following Lemma rules this out and thereby closes the gap in the proof of the theorem. ●

Lemma 6.3: Suppose that $1\notin\Sigma(\mathscr{G}^2)$ and $1\in\Sigma(\mathscr{G}^{\#2})$ with $(\mathbb{1}\pm\mathscr{G}^\#)z_\pm=0$, $z_\pm\neq 0$. Then $\langle z_\pm,\mathsf{G}^\#\rangle_+(\theta)\not\equiv 0$.

We must now prove Lemmas 6.1, 6.2, and 6.3.

Proof of Lemma 6.1: By Lemma 2.6.14 of Ref. 5 the generalized Marchenko equation always has a solution. Furthermore, if $1\notin\Sigma(\mathscr{G}^{\#2})$, where $\Sigma(\mathscr{G}^{\#2})$ is the spectrum of $\mathscr{G}^{\#2}$, then the Fourier transform of every solution of the generalized Marchenko equation

$$(\mathbb{1}\mp\mathscr{G})\Gamma_\pm=\pm\mathsf{G}_\pm,$$

$\Gamma=\Gamma_++\Gamma_-$, $F=\mathbb{1}+\int_0^\infty d\alpha\, e^{ik\alpha}\Gamma(\alpha)$, solves $W^1_0(S)$, by Lemma 2.6.12 of Ref. 5.

Now $\mathscr{G}$ is related to S precisely as $\mathscr{G}^\#$ is to $S^\#$. Suppose, then that $W^1_\sigma(S)$ has a unique solution; then it follows that $1\notin\Sigma(\mathscr{G}^2)$ and hence $W^1_0(S^\#)$ has a solution. ●

Proof of Lemma 6.2: $F_1^\#=QS^\#F_1Q$ and $F_2^\#=QSF_2Q$ imply that $\tilde{F}_1^\#F_2^\#=Q\tilde{F}_1F_2Q$. Since the left-hand side is meromorphic in $\mathbb{C}^-$ and the right-hand side in $\mathbb{C}^+$ it follows by Liouville's theorem that

$$\tilde{F}_1F_2=\mathbb{1}+\sum_j\left(\frac{R_j}{k-i\kappa_j}-\frac{QR_jQ}{k+i\kappa_j}\right):=R(k),$$

where the sum is over the (finite number of) poles specified in σ and R_j is the residue of $\tilde{F}_1F_2$, which has a finite-dimensional range. Thus there is a finite-dimensional subspace that contains the range of $R-\mathbb{1}$ for all k; hence, R is equivalent to a finite-dimensional matrix. It follows that R^{-1} is a meromorphic function of k and hence $\tilde{F}_1$ has a meromorphic right inverse I_R with $I_R-\mathbb{1}\in\mathscr{M}^+$.

On the other hand, $\lim_{|k|\to\infty}\|F_1-\mathbb{1}\|=0$, which implies that for $|k|$ sufficiently large, $\tilde{F}_1$ has a holomorphic inverse. This inverse, being equal to F_2R^{-1} in an open set, can be analytically continued to all of $\mathbb{C}^+$. Hence, $\tilde{F}_1$ and F_1 have inverses that are meromorphic in $\mathbb{C}^+$ with a finite number of poles. It follows similarly that F_2 has a meromorphic inverse. ●

Proof of Lemma 6.3: Note that it follows from

$$z_\pm(\alpha,\theta)=\mp\int_0^\infty d\beta\int_{S^2}d\theta'\,G(-\alpha-\beta,\theta,\theta')z_\pm(\beta,\theta'),\tag{21}$$

for $\alpha\geqslant 0$, in the limit as $\alpha\to 0$ that

$$z_\pm(0,\theta)=\mp\int_0^\infty d\beta\int_{S^2}d\theta'G(-\beta,\theta,\theta')z_\pm(\beta,\theta')$$

and hence $\langle z_\pm,\mathsf{G}^\#\rangle_+\equiv 0$ is equivalent to $z_\pm(0,\theta)=0$ for almost all $\theta\in S^2$ if $(\mathbb{1}\pm\mathscr{G}^\#)z_\pm=0$.

Suppose first that for *all* nontrivial solutions $z_\pm$ of $(\mathbb{1}\pm\mathscr{G}^\#)z_\pm=0$ we have $\langle z_\pm,\mathsf{G}^\#\rangle_+\equiv 0$. Let $z_\pm$ be such a nontrivial solution. Differentiate (21) with respect to α, calling $z'_\pm(\alpha,\theta):=\partial/\partial\alpha z_\pm(\alpha,\theta)$, and integrate by parts:

$$\begin{aligned}z'_\pm(\alpha,\theta)&=\mp\int_0^\infty d\beta\int_{S^2}d\theta'\frac{\partial}{\partial\beta}G(-\alpha-\beta,\theta,\theta')z_\pm(\beta,\theta')\\&=\pm\int_0^\infty d\beta\int_{S^2}d\theta'G(-\alpha-\beta,\theta,\theta')z'_\pm(\beta,\theta'),\end{aligned}$$

which means that $(\mathbb{1}\mp\mathscr{G}^\#)z'_\pm=0$. Since $z_\pm(0,\theta)\equiv 0$, $z'_\pm\equiv 0$ would imply $z_\pm\equiv 0$, which is not the case, by assumption; therefore $z'_\pm$ does not vanish identically and $(\mathbb{1}\mp\mathscr{G}^\#)z'_\pm=0$. Now, since by assumption $\langle z,\mathsf{G}^\#\rangle_+\equiv 0$ for all solutions of $(\mathbb{1}\pm\mathscr{G}^\#)z=0$, it follows that $z'_\pm(0,\theta)\equiv 0$ and we may repeat the argument for the second derivative, and so on. Let us concentrate on z_+.

Since the null space of $(\mathbb{1}+\mathscr{G}^\#)$ is finite-dimensional, the derivatives of z_+ must eventually become linearly dependent and we must have two linear relations of the form

$$\sum_{n=0}^N c_n^{(1)}z_+^{(2n)}(\alpha,\theta)=0,$$

$$\sum_{n=0}^N c_n^{(2)}z_+^{(2n+1)}(\alpha,\theta)=0,$$

and also $z_+^{(n)}(0,\theta)\equiv 0$, $n=0,\ldots,2N$, where $z_+^{(n)}:=\partial^n z_+/\partial\alpha^n$. These systems have only the trivial solution $z_+(\alpha,\theta)=0$. Similarly, for $z_-(\alpha,\theta)=0$. We conclude that it is impossible that *all* solutions of $(\mathbb{1}\pm\mathscr{G}^\#)z_\pm=0$ satisfy $\langle z_\pm,\mathsf{G}^\#\rangle_+\equiv 0$.

Suppose next that for *one* solution we have $\langle z_+,\mathsf{G}^\#\rangle_+\not\equiv 0$. Let $\{z_\pm^{[n]}\}$, $n=1,\ldots,N$, be orthogonal basis sets in $\mathrm{nul}(\mathbb{1}\pm\mathscr{G}^\#)$ so that $\langle z_+^{[1]},\mathsf{G}^\#\rangle_+\not\equiv 0$, $\langle z_-^{[1]},\mathsf{G}^\#\rangle_+\equiv 0$, and $\langle z_\pm^{[n]},\mathsf{G}^\#\rangle_+\not\equiv 0$, $n>1$. If we pose $W^1_\sigma(S)$ with $n_\sigma=1$ then Eq. (13) can always be solved for any given $\mathscr{Y}$, since $1\notin\Sigma(\mathscr{G}^2)$. For $n_\sigma=1$ we have $\mathscr{Y}_\pm=y\rho_\pm$ and Eqs. (15) with (11) and (12) read

$$\langle z_+^{[1]},\mathsf{G}^\#_+\rangle_+=2\langle z_+^{[1]},y\rangle_+\rho_+,$$

$$0=\langle z_-^{[1]},y\rangle_+\rho_-,$$

$$0=\langle z_\pm^{[n]},y\rangle_+\rho_\pm,\quad n>1.$$

Therefore, if y is chosen so that $\langle z_+^{[1]},y\rangle_+\neq 0$, $\langle z_-^{[1]},y\rangle_+\neq 0$, and $\langle z_\pm^{[n]},y\rangle_+=0$, $n>1$, (which is always possible) then $\rho_\pm$ is uniquely determined and the solution of (13) leads to a unique solution of $W^1_\sigma(S)$ with $n_\sigma=1$. The same would be true if we had chosen $\langle z_-,\mathsf{G}^\#\rangle_+\not\equiv 0$ instead of $\langle z_+,\mathsf{G}^\#\rangle_+\not\equiv 0$.

Next, suppose that $n_\sigma=2$. Then $\mathscr{Y}_\pm=y^{[1]}\rho_\pm^{[1]}+y^{[2]}\rho_\pm^{[2]}$ leads to

$$\sum_{j=1}^{2} s_{ij}^{\pm}\rho_{\pm}^{[j]} = c_i^{\pm}, \quad i=1,2,$$

where

$$s_{ij}^{\pm} := \langle z_{\pm}^{[i]}, y^{[j]} \rangle_{+}, \quad c_1^{\pm} := \langle z_{\pm}^{[1]}, \mathsf{G}_{\pm}^{\#} \rangle_{+} \not\equiv 0,$$
$$c_2^{\pm} = \langle z_{\pm}^{(2)}, \mathsf{G}_{\pm}^{\#} \rangle_{+} \equiv 0.$$

If the functions $y^{[i]}$, $i=1,2$, are chosen in such a way that $\det s^{\pm} \neq 0$, then the $\rho_{\pm}^{[i]}$ are uniquely determined. They also satisfy the remaining equations if the $y^{[i]}$ are chosen so that $\langle z_{\pm}^{[i]}, y^{[j]} \rangle_{+} = 0$, $i>2$, $j=1,2$. The final constraint on the $y^{[i]}$ is that $(s_{\pm}^{-1})_{i1} \neq 0$, $i=1,2$, so that $\rho_{\pm}^{[i]} \not\equiv 0$, $i=1,2$. The large class from which the functions y may be chosen make such choices always possible. Thus we get a unique solution of $W_{\sigma}^{1}(S)$ with $n_{\sigma}=2$ as well as a unique solution of $W_{\mu}^{1}(S)$ with $n_{\mu}=1$. Since $1 \notin \Sigma(\mathscr{G}^2)$ it follows from Lemma 2.6.14 of Ref. 5 that $W_0^1(S^{\#})$ has a solution. [Remember that $\mathscr{G}$ corresponds to S as $\mathscr{G}^{\#}$ does to $S^{\#}$.] Therefore, by Lemma 6.2, the solutions of $W_{\sigma}^{1}(S)$ and $W_{\mu}^{1}(S)$ are meromorphically invertible. It then follows from Lemma 2.6.8 of Ref. 5 that this is impossible: Two problems with unequal numbers of poles cannot both be uniquely solvable. Therefore, it cannot be the case that $\langle z_{\pm}, \mathsf{G}^{\#} \rangle_{+} \equiv 0$ for all but one $z_{\pm}$. Similar arguments rule out any other number, and we may conclude that for all $z_{\pm}$ we must have $\langle z_{\pm}, \mathsf{G}^{\#} \rangle_{+} \not\equiv 0$. ●

Proof of Lemma 3.2: We shall fix our attention on s^{+} and z_{+}, leaving off the $+$; the same argument holds for $-$. Let $n = \dim \operatorname{nul}(1+\mathscr{G}^{\#})$. The equation $sa=0$ means that $\langle z_r, \tilde{y}a \rangle_{+} = 0$ for all $1 \leqslant r \leqslant n$, i.e., there exists a linear combination of n functions y_m^b as in (10), with given numbers κ_m, that lies in $\Omega := [\operatorname{nul}(1+\mathscr{G}^{\#})]_{\perp} = \operatorname{ran}(1+\mathscr{G}^{\#})$. Assume that the lemma is false. Then, no matter how the n functions $Y_{\kappa_m}^b$ are chosen, there always exists such a linear combination. So choose an arbitrary set of n functions $Y_{\kappa_m}^b$; then $\exists \{a_{mb}\}$ such that

$$\sum_{m,b} a_{mb} Y_{\kappa_m}^b e^{-\alpha\kappa_m} \in \Omega.$$

Now choose another arbitrary set, but with one of the functions $Y_{\kappa_m}^b$ the same as before; again, $\exists \{a'_{mb}\}$ such that

$$\sum_{m,b} a'_{mb} Y_{\kappa_m}^b e^{-\alpha\kappa_m} \in \Omega.$$

It follows by subtraction that for any arbitrary set of one member less than before, $\exists \{a''_{mb}\}$ such that

$$\sum_{m,b} a''_{mb} Y_{\kappa_m}^b e^{-\alpha\kappa_m} \in \Omega.$$

This process is repeated until we arrive at the statement that for any arbitrary function Y_{κ}^b and any arbitrary κ:

$$Y_{\kappa}^b(-\theta) e^{-\alpha\kappa} \in \Omega.$$

But these functions span all of $L^2(\mathbb{S}^2 \times \mathbb{R}_{+})$; hence $L^2(\mathbb{S}^2 \times \mathbb{R}_{+}) \subset \Omega$ is implied, which is false since $\operatorname{codim} \Omega = n$. This proves the lemma. ●

Proof of Lemma 4.2: It follows from the well-known formula

$$\operatorname{tr}\left[\frac{dS}{dk} S^{-1}\right] = \frac{d}{dk} \ln \det S$$

that if the eigenvalues of S are $e^{2i\eta_n}$ then

$$\operatorname{tr} \int_{-\infty}^{\infty} dk\, S'(k) S^{-1}(k)$$
$$= 2i \sum_n \int_{-\infty}^{\infty} dk\, \eta_n'(k) = 4i \sum_n [\eta_n(k)]_0^{\infty}$$
$$= -4i \sum_n \eta_n(0) = -4i\delta(0) = -4\pi i \operatorname{ind}_{\mathrm{L}} S,$$

since $S(-k) = \bar{S}(k)$ and by the definition of the Levinson index. Now if $S = QS^{\#-1}Q$ and it has a left standard factorization then the factorization can be chosen so that $W_{-} = QW_{+}^{\#-1}$ (Ref. 10). Then

$$\operatorname{tr} \int_{-\infty}^{\infty} dk\, S' S^{-1}$$
$$= \operatorname{tr} \int_{-\infty}^{\infty} dk\, D' D^{-1} + \operatorname{tr} \int_{-\infty}^{\infty} dk\, W'_{+} W_{+}^{-1}$$
$$+ \operatorname{tr} \int_{-\infty}^{\infty} dk\, W'_{-} W_{-}^{-1}$$
$$= \operatorname{tr} \int_{-\infty}^{\infty} dk\, D' D^{-1} + 2 \operatorname{tr} \int_{-\infty}^{\infty} dk\, W'_{+} W_{+}^{-1},$$

and by closing the contour of integration in the upper half-plane it follows from the analyticity and asymptotics of W_{+} that

$$\int_{-\infty}^{\infty} dk\, W'_{+} W_{+}^{-1}$$
$$= [W_{+}(k)]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dk\, W'_{+} [W_{+}^{-1} - 1] = 0.$$

On the other hand one readily computes from the form (5) of D that

$$\operatorname{tr} \int_{-\infty}^{\infty} dk\, D' D^{-1} = -2\pi i \sum \rho_j.$$

As a result we have

$$\operatorname{tr} \int_{-\infty}^{\infty} dk\, S' S^{-1} = -2\pi i \operatorname{ind}_{\mathrm{WH}} S,$$

a formula that was first given by Gohberg and Leiterer in Ref. 14. It follows that $\operatorname{ind}_{\mathrm{L}} S = \frac{1}{2} \operatorname{ind}_{\mathrm{WH}} S$. (It would be desirable to find a more rigorous proof that is based on specific properties of S and of V if S is admissible.) ●

Proof of Lemma 4.3: Suppose that σ is an eigenfunction of $\mathscr{G}^{\#}$ with the eigenvalue -1. Then its Fourier transform f solves $W_0^0(-S)$ and satisfies the equation $f^{\#} = -QSf$. Use this function to define

$$\varphi(k,x) := \int d\theta\, f(k,\theta) \psi(k,\theta,x),$$

where ψ is the outgoing-wave solution of the Schrödinger equation and the integral extends over $\mathbb{S}^2$. It follows that φ is a solution of the Schrödinger equation that is an odd function of k, and if there are no bound states (which we shall assume to begin with), it is an entire analytic function of k that is $o(|k|r)$ as $|k| \to \infty$, where $r = |x|$. By the Paley–Wiener theorem its Fourier transform vanishes for $|t| > r$ and it may be written in the form

$$\varphi(k,x)=\int_{-r}^{r} dt\, s(t,x)\sin kt\,.$$

Use of the Schrödinger equation and two integrations by parts lead to the hyperbolic partial differential equation

$$\left[\Delta-\frac{\partial^2}{\partial t^2}-V(x)\right]s=0,\quad t>-|x|\,. \tag{22}$$

Furthermore, we must have

$$s(-r,x)=0,\quad \lim_{r\to\infty} s(t,x)=0\,. \tag{23}$$

This quasi-Goursat problem has only the trivial solution. An outline of the proof (the details of which will be given in a subsequent paper) of this assertion is as follows.

One first proves that the system

$$\left[\Delta-\frac{\partial^2}{\partial t^2}\right]g=0,\quad x\in\mathbb{R}^3,\quad t>-|x|\,, \tag{24}$$

$$g|_{t\to-|x|}=g|_{|x|\to\infty}=0\,, \tag{25}$$

has only the trivial solution. This, in turn, is proved by expanding the angle dependence of g on spherical harmonics and proving that the system

$$\left[\frac{\partial^2}{\partial r^2}-\frac{\partial^2}{\partial t^2}-\frac{l(l+1)}{r^2}\right]g_l=0,\quad t>r,\quad r>0\,,$$

$$g_l|_{t\to-r}=g_l|_{r\to\infty}=0\,,$$

has only the trivial solution.

The case with $V\neq 0$ is then proved by assuming that s satisfies the system (22), (23) and setting $s=0$ for $t<-|x|$. Then the function

$$F(t,x):=s(t,x)+\int dy\,\frac{V(y)}{4\pi|x-y}\,s(t-|x-y|,y)$$

is seen to satisfy the system (24), (25) and hence must vanish. Therefore, s satisfies a homogeneous integral equation the Fourier transform (with respect to t) of which is the homogeneous form of the Lippmann–Schwinger equation. It follows that $s=0$. Consequently, $\varphi(k,x)=0$ and hence $f(k,\theta)=0$, contrary to assumption. Therefore, if V causes no bound states then $\mathcal{G}^{\#}$ cannot have the eigenvalue -1.

Consider now the case with bound states. In that case the function φ has simple poles at the points $k=i\kappa_n$ with residues $\Sigma_b h^b_\kappa u^b_\kappa(x)$, where $u^b_\kappa(x)$ is a bound state eigenfunction of the Schrödinger equation with the eigenvalue $-\kappa_n^2$ and

$$h^b_\kappa:=\int d\theta\, f(i\kappa,\theta)\,Y^b_\kappa(-\theta), \tag{26}$$

Y^b_κ being a bound state character. Now the Fourier transform of φ is

$$s(t,x)=\frac{i}{\pi}\int_{-\infty}^{\infty} dk\, e^{-ikt}\varphi(k,x).$$

When $t>r$ the contour may be closed by a large semicircle in the lower half-plane and one obtains

$$s(t,x)=2\sum_{b,\kappa_m} h^b_{\kappa_m}u^b_{\kappa_m}(x)e^{-\kappa_m t}:=s_0(t,x). \tag{27}$$

Therefore,

$$\varphi(k,x)=\int_0^r dt\,\sin kts(t,x)+\int_r^\infty dt\,\sin kts_0(t,x).$$

Insertion of φ in the Schrödinger equation now results in the hyperbolic equation for $-r\leqslant t\leqslant r$

$$\left[\Delta-\frac{\partial^2}{\partial t^2}-V\right]s=0,$$

$s(-t,x)=-s(t,x)$, and the boundary condition at $t=r,(\partial/\partial r)\{r[s(r,x)-s_0(r,x)]\}=0$, which implies that $s(r,x)=s_0(r,x)$. The earlier argument shows that the solution of this problem is unique.

Suppose that there are N bound states. Then there are N linearly independent functions u^b_κ and hence N linearly independent functions $s_0(t,x)$. This leads to exactly N linearly independent solutions $s(t,r)$ because the previous argument showed that $s_0=0$ implies $s=0$. But the number of linearly independent functions s equals the number of linearly independent functions φ, which, in turn, equals the number of linearly independent functions f, the Fourier transforms of eigenfunctions of $\mathcal{G}^{\#}$ with the eigenvalue -1. Therefore, the total number of eigenvalues of the Schrödinger equation, counting their degeneracy, equals the dimension of the eigenspace of $\mathcal{G}^{\#}$ at the eigenvalue -1.

The proof for the eigenvalue $+1$ is the same, except that then $s(t,x)$ is an even function of t and sin kt is replaced by cos kt. ●

Proof of Lemma 4.4: Assume that s^+ is not invertible. This implies that there exists a set of N complex numbers a_n such that $\Sigma_n a_n s^+_{n,mb}=0$ for all N values of the pair m,b. Hence, there is a vector $z=\Sigma_n a_n z^{[n]}_+\in\mathrm{nul}(\mathbf{1}+\mathcal{G}^{\#})$ such that

$$\langle z,y^b_m\rangle_+=0 \tag{28}$$

for all y^b_m defined by (10). Let $f(k,\theta)$ be the Fourier transform of z. A short calculation shows that (28) is equivalent to

$$\int_{S^2} d\theta\, Y^b_{\kappa_m}(-\theta)f(i\kappa_m,\theta)=0$$

for all $\kappa_m\in\mathbf{P}_\sigma$ and all the character functions $Y^b_{\kappa_m}$. We take this f to be the function used in the proof of Lemma 4.3. Then it follows that all the functions $h^b_{\kappa_m}$ defined by (26) vanish. Consequently, s_0 of (27) vanishes, and hence by the first part of the proof of Lemma 4.3 we have $s(t,x)=0$ and, hence, $f=0$ and $z=0$, contrary to our initial assumption. The proof that s^- is invertible is similar. ●

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Anisotropic homogeneous cosmologies with perfect fluid and electric field

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A new three-parameter family of cosmological models is found, which are solutions of Einstein–Maxwell equations in a space-time filled with electrically neutral stiff matter. They generalize an anisotropic homogeneous cosmology without electromagnetic field by Vajk and Eltgroth [J. Math. Phys. **11**, 2212 (1970)] and support a conjecture about proportionality of electromagnetic four-potential of an Einstein–Maxwell solution and the Killing vector of a corresponding space-time with stiff matter. This conjecture turns out to be the clue to a new solution-generating method of Einstein–Maxwell fields with sources.

I. INTRODUCTION

A new method of generation of electrovacuum solutions in general relativity was proposed recently by Horský and Mitskiévic.[1] This method does not remove the necessity of solving Einstein's equations, but it simplifies (sometimes quite considerably) the manipulations with Maxwell's equations, reducing them, in fact, to a certain kind of condition (we call them Maxwell's conditions). It is applicable to vacuum seed solutions of Einstein's equations possessing at least one isometry (in contrast with many other methods that depend on the existence of two Killing vectors).

We propose now a generalization of this method to a case when the seed solution (still possessing one isometry as a minimum) corresponds not to a vacuum, but to a stiff perfect fluid ($p=\mu$). The resulting self-consistent system includes gravitational and electromagnetic fields, as well as electrically neutral stiff matter.

In Sec. II we discuss the main ideas of the generation method (as well as of its further generalizations). In Sec. III we generate a new three-parameter family of metrics by applying this method to a specific seed solution, namely to that found by Vajk and Eltgroth.[2] These authors have also presented superpositions of a magnetic field and perfect fluid, but not in the case when $p=\mu$; moreover, our solutions show greater anisotropy than those considered by them, even when the electric field is switched off. The latter subcase as well as other limiting cases are considered in Sec. IV. In the same section we determine the Petrov types of our solutions. A final discussion of the results is given in Sec. V.

Greek indices run from 0 to 3, the space-time signature is $(+\ -\ -\ -)$.

II. TEST ELECTROMAGNETIC FIELDS ON THE BACKGROUND OF SPACE-TIMES WITH ISOMETRIES AND TRANSITION TO A SELF-CONSISTENT SYSTEM

On the background of a space-time admitting a Killing vector ξ, we consider an electromagnetic field with four-potential $A=k\xi$ that satisfies the usual Lorenz condition,[3] $A^{\alpha}{}_{;\alpha}=0$ (k is an arbitrary constant). Then, by virtue of the properties of Killing vectors,

$$F^{\mu\nu}_{\ ;\nu}=(A^{\nu;\mu}-A^{\mu;\nu})_{;\nu}=2k\xi_{\nu}{}^{;\mu;\nu}=-2k\xi^{\lambda}R_{\lambda\mu}$$
$$=2k\kappa\xi^{\lambda}\left(T_{\lambda\mu}-\tfrac{1}{2}Tg_{\lambda\mu}\right)=-4\pi j_{\mu}. \tag{1}$$

In a vacuum, $T_{\mu\nu}=0$, this leads to the well-known conclusion[4] that a Killing vector of a vacuum space-time generates a test sourceless electromagnetic field on the background of the same space-time. In the case of a nonzero stress-energy tensor of a perfect fluid, $T_{\mu\nu}=(\mu+p)u_{\mu}u_{\nu}-pg_{\mu\nu}$, the test electromagnetic field corresponds to the four-current density

$$j_{\mu}=-(k\kappa/2\pi)\left[(\mu+p)u_{\lambda}\xi^{\lambda}u_{\mu}-\tfrac{1}{2}(\mu-p)\xi_{\mu}\right], \tag{2}$$

which is also a test object with respect to the space-time geometry. However, the already mentioned case of a sourceless test electromagnetic field still can be generalized to such a nonvacuum gravitational field, if two conditions are satisfied:

$$u\perp\xi \quad \text{and} \quad \mu=p. \tag{3}$$

This means that the Killing vector under consideration is spacelike and the perfect fluid (the source of the background metric) is stiff.

Otherwise we have a test electromagnetic field with sources, and, if we would like to contact them with the background perfect fluid, we have either to consider it to be stiff, or to admit the Killing vector to be proportional to the four-velocity u of the fluid (then the space-time is stationary). Below we consider only the case of a stiff matter and $\xi\perp u$.

In Ref. 1 it is noticed that the timelike Killing vectors of the Schwarzschild and Kerr fields coincide (up to a constant factor) with the electromagnetic four-potentials of the Reissner–Nordstrøm and Kerr–Newman fields, respectively, and other examples of such a correspondence are found. Thus a conjecture was formulated that a Killing covector of a seed space-time represents (up to a constant factor) an electromagnetic four-potential which belongs to a new self-consistent system of gravitational and electromagnetic fields. When the electromagnetic field is switched off (this is done by tending a parameter to zero, say, k), the initial seed metric is recovered. It is worth emphasizing that the both cases, those of the test and nontest fields, are interconnected in such a simple way only in their covariant, and not contravariant, representation, since raising indices should be performed with the help of different metrics thus breaking the similarity between corresponding quantities.

In solving the problem of generation of Einstein–Maxwell fields on the basis of this conjecture, further steps in-

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volve some natural assumptions as to the structure of the new metric. Usually, it is merely enough to introduce some new functions, which are to be determined by solving Einstein's equations (instead of the functions already existing in the seed metric, but without changing the general structure of it).

In the following section a detailed example is given that shows how this new method of generation of Einstein–Maxwell fields works.

III. COSMOLOGY WITH A SUPERPOSITION OF NEUTRAL STIFF MATTER AND ELECTRIC FIELD

We shall now apply our method to a seed solution obtained by Vajk and Eltgroth,[2,5]

$$ds^2 = dt^2 - t^{2/(1+2\lambda)}\,dx^2 - t^{2\lambda/(1+2\lambda)}\,dy^2 - t^{2\lambda/(1+2\lambda)}\,dz^2, \tag{4}$$

where λ is a free parameter, $\lambda > 0$ or $\lambda < -2$. Then the stress-energy tensor corresponds to a stiff matter with

$$\mu = p = (2+\lambda)\lambda/\kappa_0(1+2\lambda)^2 t^2. \tag{5}$$

Here we shall make use of one of the (spacelike) Killing vectors of the solution (4), $\xi = -\partial_y$, or, as a one-form, $\xi = t^{2\lambda/(1+2\lambda)}\,dy$, thus taking a four-potential covector

$$A = k\xi = kt^{2\lambda/(1+2\lambda)}\,dy, \quad k = \text{const.} \tag{6}$$

Since the conditions (3) are satisfied, this field is a solution of sourceless Maxwell equations on the background of the metric (4): this is our test electromagnetic field. The covector (6) can be brought to a simpler form,

$$A = kt\,dy, \tag{7}$$

by another choice of the coordinate t. Then the Maxwell tensor becomes

$$\tfrac{1}{2} F_{\mu\nu}\,dx^\mu \wedge dx^\nu = k\,dt \wedge dy. \tag{8}$$

Let us now consider a generalized metric

$$ds^2 = e^{2\alpha}\,dt^2 - e^{2\beta}\,dx^2 - e^{2\gamma}\,dy^2 - e^{2\delta}\,dz^2, \tag{9}$$

where α, β, γ, and δ are functions of the coordinate t, that leads to a natural orthonormal tetrad,

$$\theta^{(0)} = e^\alpha\,dt, \quad \theta^{(1)} = e^\beta\,dx, \quad \theta^{(2)} = e^\gamma\,dy, \quad \theta^{(3)} = e^\delta\,dz. \tag{10}$$

In this space-time,

$$\tfrac{1}{2} F^{\mu\nu}\partial_\mu \otimes \partial_\nu = ke^{-2\alpha-2\gamma}\partial_{[y} \otimes \partial_{t]}, \tag{11}$$

so that Maxwell's equations are supposed to yield

$$\frac{d}{dt}\left(e^{-\alpha+\beta-\gamma+\delta}\right) = 0$$

in agreement with the property of the Killing field ξ on the background of the seed metric (4), and as a result of the Horský–Mitskiévic conjecture. This is equivalent to

$$e^{-\alpha+\beta-\gamma+\delta} = A = \text{const}, \tag{12}$$

which we call Maxwell's condition, with $A = 1$ (without any loss of generality). Now, the electromagnetic field invariant

$$F_{\mu\nu}F^{\mu\nu} = -2k^2 e^{-2\alpha-2\gamma}$$

being negative, this is an electric-type field, not a magnetic-type one.

Components of the stress-energy tensor of this electric field with respect to the orthonormal tetrad (10),

$$T^e_{(\mu)(\nu)}\theta^{(\mu)} \otimes \theta^{(\nu)} = (k^2/8\pi)e^{-2\alpha-2\gamma}[\theta^{(0)} \otimes \theta^{(0)} + \theta^{(1)} \otimes \theta^{(1)} - \theta^{(2)} \otimes \theta^{(2)} + \theta^{(3)} \otimes \theta^{(3)}], \tag{13}$$

reflects the minimal possible anisotropy of the space-time geometry under consideration. When $k = 0$, the electric field is switched off.

The tetrad choice (10) leads to the following curvature two-forms:

$$\begin{aligned}
\Omega^{(0)}{}_{(1)} &= e^{-2\alpha}(\ddot{\beta} + \dot{\beta}^2 - \dot{\alpha}\dot{\beta})\theta^{(0)} \wedge \theta^{(1)},\\
\Omega^{(0)}{}_{(2)} &= e^{-2\alpha}(\ddot{\gamma} + \dot{\gamma}^2 - \dot{\alpha}\dot{\gamma})\theta^{(0)} \wedge \theta^{(2)},\\
\Omega^{(0)}{}_{(3)} &= e^{-2\alpha}(\ddot{\delta} + \dot{\delta}^2 - \dot{\alpha}\dot{\delta})\theta^{(0)} \wedge \theta^{(3)},\\
\Omega^{(1)}{}_{(2)} &= \dot{\beta}\dot{\gamma}e^{-2\alpha}\theta^{(1)} \wedge \theta^{(2)},\\
\Omega^{(1)}{}_{(3)} &= \dot{\beta}\dot{\delta}e^{-2\alpha}\theta^{(1)} \wedge \theta^{(3)},\\
\Omega^{(2)}{}_{(3)} &= \dot{\gamma}\dot{\delta}e^{-2\alpha}\theta^{(2)} \wedge \theta^{(3)},
\end{aligned} \tag{14}$$

(differentiation with respect to t is denoted by an overdot).

The stress-energy tensor of a stiff matter ($\mu = p$) has the form

$$T^m_{(\alpha)(\beta)}\theta^{(\alpha)} \otimes \theta^{(\beta)} = p[\theta^{(0)} \otimes \theta^{(0)} + \theta^{(1)} \otimes \theta^{(1)} + \theta^{(2)} \otimes \theta^{(2)} + \theta^{(3)} \otimes \theta^{(3)}], \tag{15}$$

where p is the proper stress (and the proper density) of the perfect fluid.

Einstein's equations then read

$$e^{-2\alpha}(\dot{\beta}\dot{\gamma} + \dot{\beta}\dot{\delta} + \dot{\gamma}\dot{\delta}) = \kappa(p + (k^2/8\pi)e^{-2\alpha-2\gamma}), \tag{16a}$$

$$e^{-2\alpha}(\dot{\alpha}\dot{\gamma} + \dot{\alpha}\dot{\delta} - \dot{\gamma}\dot{\delta} - \ddot{\gamma} - \dot{\gamma}^2 - \ddot{\delta} - \dot{\delta}^2) = \kappa(p + (k^2/8\pi)e^{-2\alpha-2\gamma}), \tag{16b}$$

$$e^{-2\alpha}(\dot{\alpha}\dot{\beta} + \dot{\alpha}\dot{\delta} - \dot{\beta}\dot{\delta} - \ddot{\beta} - \dot{\beta}^2 - \ddot{\delta} - \dot{\delta}^2) = \kappa(p - (k^2/8\pi)e^{-2\alpha-2\gamma}), \tag{16c}$$

$$e^{-2\alpha}(\dot{\alpha}\dot{\beta} + \dot{\alpha}\dot{\gamma} - \dot{\beta}\dot{\gamma} - \ddot{\beta} - \dot{\beta}^2 - \ddot{\gamma} - \dot{\gamma}^2) = \kappa(p + (k^2/8\pi)e^{-2\alpha-2\gamma}). \tag{16d}$$

Maxwell's condition (12) and Einstein's equations (16) form a self-consistent system that is equivalent to the system of the Einstein–Maxwell equations. Next, we consider the subtraction of these equations from one another:

$$e^{-2\alpha}[e^{-\alpha+\beta+\gamma+\delta}(\dot{\delta} - \dot{\gamma})]^{\cdot} = (\kappa k^2/4\pi)e^{-3\alpha+\beta-\gamma+\delta}, \tag{16c-d}$$

$$[e^{-\alpha+\beta+\gamma+\delta}(\dot{\gamma} + \dot{\delta})]^{\cdot} = 0, \tag{16a-b}$$

$$[e^{-\alpha+\beta+\gamma+\delta}(\dot{\beta} + \dot{\gamma})]^{\cdot} = 0. \tag{16a-d}$$

Inserting Maxwell's conditions (12) into these equations, we obtain

$$e^{2\gamma} = -(\kappa k^2/8\pi)t^2 + Bt + C, \tag{17}$$

$$e^{2\beta} = G\left(-\frac{\kappa k^2}{8\pi}t^2 + Bt + C\right)^{-1} \times\left\{C^{\operatorname{sgn} B}\left(-\frac{\kappa k^2}{4\pi}t + B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right. \times\left.\left[\left(-\frac{\kappa k^2}{4\pi}t + B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right]^{-1}\right\}^{(2F+B)/\sqrt{B^2 + (\kappa k^2/2\pi)C}}, \tag{18}$$

$$e^{2\delta} = E\left(-\frac{\kappa k^2}{8\pi}t^2 + Bt + C\right)^{-1} \times\left\{C^{\operatorname{sgn} B}\left(-\frac{\kappa k^2}{4\pi}t + B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right. \times\left.\left[\left(-\frac{\kappa k^2}{4\pi}t + B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right]^{-1}\right\}^{(2D+B)/\sqrt{B^2 + (\kappa k^2/2\pi)C}}, \tag{19}$$

$$e^{2\alpha} = \frac{EG}{A^2}\left(-\frac{\kappa k^2}{8\pi}t^2 + Bt + C\right)^{-3} \times\left\{C^{\operatorname{sgn} B}\left(-\frac{\kappa k^2}{4\pi}t^2 + B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right. \times\left.\left[\left(-\frac{\kappa k^2}{4\pi}t + B + \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\left(B - \sqrt{B^2 + \frac{\kappa k^2}{2\pi}C}\right)\right]^{-1}\right\}^{2(D+F+B)/\sqrt{B^2 + (\kappa k^2/2\pi)C}}. \tag{20}$$

Taking another choice of the integration constants we represent our solution in a simpler form:

$$e^{2\alpha} = (MN/A^2C)(\tilde{\sigma}t + 1)^{n+m-3}(\tilde{\tau}t + 1)^{-n-m-3},$$
$$e^{2\beta} = N(\tilde{\sigma}t + 1)^{n-1}(\tilde{\tau}t + 1)^{-n-1},$$
$$e^{2\gamma} = C(\tilde{\sigma}t + 1)(\tilde{\tau}t + 1),$$
$$e^{2\delta} = M(\tilde{\sigma}t + 1)^{m-1}(\tilde{\tau}t + 1)^{-m-1}. \tag{21}$$

Then

$$ds^2 = (MN/A^2C)(\tilde{\sigma}t + 1)^{n+m-3}(\tilde{\tau}t + 1)^{-n-m-3}dt^2 - N(\tilde{\sigma}t + 1)^{n-1}(\tilde{\tau}t + 1)^{-n-1}dx^2 - C(\tilde{\sigma}t + 1)(\tilde{\tau}t + 1)dy^2 - M(\tilde{\sigma}t + 1)^{m-1}(\tilde{\tau} + 1)^{-m-1}dz^2. \tag{22}$$

A final transformation and rescaling of the metric (22) yield

$$ds^2 = T^{-n-m-3}(b - aT)^{n+m-3}dT^2 - T^{-n-1}(b - aT)^{n-1}dx^2 - T(b - aT)dy^2 - T^{-m-1}(b - aT)^{m-1}dz^2. \tag{23}$$

Here a and b are constant parameters satisfying the conditions

$$b = 1 + a, \quad a = \kappa k^2/8\pi \geqslant 0, \tag{24}$$

so that $b \geqslant 1$.

We now obtain for the proper stress in (15), for the electrically neutral stiff matter,

$$p = [b^2(mn - 1)/4\kappa]T^{n+m+1}(b - aT)^{-n-m+1}, \tag{25}$$

and for the electromagnetic field invariant,

$$F_{(\mu)(\nu)}F^{(\mu)(\nu)} = -(16\pi/\kappa)aT^{n+m+2}(b - aT)^{-n-m+2}. \tag{26}$$

IV. LIMITING CASES AND THE PETROV CLASSIFICATION OF THE NEW SPACE-TIME

We consider first the case when $a = 0$ (the electric field being switched off). Then the metric (23) takes the form

$$ds^2 = T^{-n-m-3}dT^2 - T^{-n-1}dx^2 - Tdy^2 - T^{-m-1}dz^2, \tag{27}$$

with the pressure

$$p = [(mn - 1)/4\kappa]T^{n+m+1}. \tag{28}$$

One recovers the seed metric (4) after performing a transformation

$$T = \{[(1 + 2\lambda)/2\lambda]t\}^{2\lambda/(1+2\lambda)},$$

and assigning to m and n the values $m = -2$, $n = -(1 + 1/\lambda)$; corresponding rescalings of x, y, and z are to be performed simultaneously. The new solution (27) is more general than the metric (4): In our new space-time a complete spatial anisotropy is present even in the absence of an electric field. Moreover, one can also "switch off" the perfect fluid by putting $mn = 1$, which leads to $\mu = p = 0$, leaving us with a mere vacuum. The resulting metric,

$$ds^2 = T^{-n-(1/n)-3}dT^2 - T^{-n-1}dx^2 - Tdy^2 - T^{-(1/n)-1}dz^2, \tag{29}$$

coincides with the Kasner solution.

One may, on the other hand, keep a nonvanishing elec-

tric field but put $mn = 1$; then the stiff matter disappears, and only the electric field is retained.

Of course, all the cases with electric field without sources can be reformulated to the corresponding cases with magnetic field (dual to the initial electric one) or mixtures of the both fields (duality rotation!), since the electromagnetic stress-energy tensor is the same in all these cases. Originally, Vajk and Eltgroth[2] did consider the case of a magnetic field (but not with the stiff matter as we do here).

We now apply the Petrov classification procedure as outlined in Ref. 5; the first step is to calculate the Weyl tensor components. In the orthonormal tetrad (10) the Riemann curvature components (14) yield

$$C_{(0)(3)(0)(3)} = C_{(2)(1)(1)(2)} = (e^{-2\alpha}/6)[\dot{\alpha}\dot{\beta} + \dot{\alpha}\dot{\gamma} - \ddot{\beta} - \dot{\beta}^2 - \dot{\beta}\dot{\delta} - \ddot{\gamma} - \dot{\gamma}^2 - \dot{\gamma}\dot{\delta} + 2(\ddot{\delta} + \dot{\delta}^2 - \dot{\alpha}\dot{\delta} + \dot{\beta}\dot{\gamma})], \tag{30a}$$

$$C_{(0)(2)(0)(2)} = C_{(3)(1)(1)(3)} = (e^{-2\alpha}/6)[\dot{\alpha}\dot{\beta} + \dot{\alpha}\dot{\delta} - \ddot{\beta} - \dot{\beta}^2 - \ddot{\delta} - \dot{\delta}^2 - \dot{\beta}\dot{\gamma} - \dot{\gamma}\dot{\delta} + 2(\ddot{\gamma} + \dot{\gamma}^2 - \dot{\alpha}\dot{\gamma} + \dot{\beta}\dot{\delta})], \tag{30b}$$

$$C_{(0)(1)(0)(1)} = C_{(3)(2)(2)(3)} = (e^{-2\alpha}/6)[\dot{\alpha}\dot{\gamma} + \dot{\alpha}\dot{\delta} - \ddot{\gamma} - \dot{\gamma}^2 - \ddot{\delta} - \dot{\delta}^2 - \dot{\beta}\dot{\gamma} - \dot{\beta}\dot{\delta} + 2(\ddot{\beta} + \dot{\beta}^2 - \dot{\alpha}\dot{\beta} + \dot{\gamma}\dot{\delta})] \tag{30c}$$

(all other independent components vanish identically). Now we pass to the Newman–Penrose (NP) basis,

$$\tilde{\theta}^{(0)} = (1/\sqrt{2})(\theta^{(0)} + \theta^{(1)}) = k,$$
$$\tilde{\theta}^{(1)} = (1/\sqrt{2})(\theta^{(0)} - \theta^{(1)}) = l, \tag{31}$$
$$\tilde{\theta}^{(2)} = \overline{\tilde{\theta}^{(3)}} = (1/\sqrt{2})(\theta^{(2)} + i\theta^{(3)}) = m,$$

in which the NP components of the Weyl tensor are

$$\tilde{C}_{(0)(1)(0)(1)} = -\tilde{C}_{(3)(2)(3)(2)} = C_{(0)(1)(0)(1)},$$
$$\tilde{C}_{(0)(2)(0)(2)} = -\tilde{C}_{(3)(1)(1)(3)} = \tilde{C}_{(0)(3)(0)(3)} = -\tilde{C}_{(2)(1)(1)(2)} = \tfrac{1}{2}(C_{(0)(2)(0)(2)} - C_{(0)(3)(0)(3)}). \tag{32}$$

The corresponding spinor Weyl coefficients take the form

$$\Psi_0 = \Psi_4 = W = \tfrac{1}{8}T^{n+m+1}(b - aT)^{-n+m+1} \times [12a^2T^2 - 2abT(m + 2n + 6) + b^2(n + 1)(m + 2)],$$
$$\Psi_2 = V = \tfrac{1}{24}T^{n+m+1}(b - aT)^{-n+m+1} \times [-12a^2T^2 + 2abT(3m + 6) - b^2(3m + mn + 2)],$$
$$\Psi_1 = \Psi_3 = 0, \tag{33}$$

when our metric coefficients (23) are substituted.

In general, if $W \neq 0$, we come to the Petrov type I, but if $W = 0$, $V \neq 0$, the space-time degenerates into the type D, and if $W = V = 0$, the space-time becomes conformally flat (type O). If $a \neq 0$, we have $W = 0$ at the instants

$$T_{\pm} = (b/12a) \times [m + 2n + 6 \pm (m^2 + 4n^2 - 8mn + 12)^{1/2}], \tag{34}$$

at all other times the Petrov type I being the case. W and V can vanish simultaneously (the Petrov type O) when either $m = n$ (case A) or at $T_1 = b/2a$ (case B). In case A, type O is realized at both times, T_+ and T_-. In case B this occurs at $T_1 = T_-$ only, and moreover, $mn = 1$; hence $p = 0$ [cf. (25)]. Thus this second case takes place for electrovacuum without any stiff matter; at the instant T_+ we have the Petrov type D since only W vanishes here, and not V. Otherwise, if it is only W that vanishes at T_+ and T_-, the space-time is instantaneously of type D there, being algebraically general at all other times. In the absence of the electric field ($a = 0$), the Petrov type does not change in time, so that type D takes place when either $n = -1$ or $m = -2$, or both, but $n \neq m$, and the Weyl tensor vanishes altogether, when $m = n$, $(n + 1)(n + 2) = 0$ (type O).

V. CONCLUDING REMARKS

The Einstein–Maxwell field (23), (24), (7) with neutral stiff matter (15), and (25) is a new exact self-consistent solution of the corresponding field equations and equations of motion. This solution demonstrates the effectiveness of the conjecture[1] that the electromagnetic four-potential of such a field (7) (divided by k) coincides with a Killing covector of the same metric when $k = 0$. This is the Killing vector (its contravariant version being ∂_y) of the metric (27) which itself generalizes the initial seed metric (4). The latter is of the Petrov type D, while the new space-time (27) (stiff matter without electromagnetic field) is algebraically general, if it is not specialized to (4) or to the cases mentioned in the final lines of the previous section.

We do not discuss here the singularities encountered in the space-times under consideration, as well as the range of determination of the variable T. They depend on a specific choice of the parameters a, m, and n in the metric (23), as do the eventual conclusions about the real existence and the finiteness of the loci $T = \pm\infty$ in the space-time (23).

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Curvature-squared cosmology in the first-order formalism

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Variation of the $R + \alpha R^2$ action with respect to independent metric and connection fields is shown to be equivalent to the metric-compatible fourth-order gravity coupled to a vector defined as a function of the trace of the energy-momentum tensor. The field equations are second order. The Friedmann cosmology based on this model is studied and it is shown to include nonsingular solutions at $t = 0$.

I. INTRODUCTION

Actions composed of the Einstein scalar curvature term plus quadratic powers of curvature and cosmological models based on these actions have been around for decades[1-10] despite the apparent increase in mathematical complexity, mainly because such theories seem to lead toward a less divergent quantum theory and a reasonable high-energy extension of the standard theory of general relativity (GR). Certain classes of these higher-order theories have been shown to yield either unitary,[11] or renormalizable[12,13] quantum theories while some others seem to be haunted by ghosts.

In general, since curvature is defined in terms of second derivatives of the metric tensor, an action with n powers of curvature yields field equations of order $2n$ if the metric is assumed to be the only dynamical field. In fact, all the good and bad properties of higher-order theories are due to the increase in the order of the field equations. Attempts have been made to exorcise these theories by going to a higher number of dimensions and adding dimensionally continued Euler-invariant combinations of higher powers of curvature such that the field equations are nevertheless second order.[14,15] Dimensionally continued Euler invariants have also been predicted in the low energy limit of some Superstring theories[16,17] and some seem to admit spontaneous compactification.[18,19]

While resorting to higher dimensions and considering Euler-invariant contributions to the Einstein action may be a promising route to take, here, we suggest an alternative route which is by no means a new one.[2,7,8] We suggest obtaining second-order equations from quadratic actions by following the Palatini formalism of treating the metric tensor and the connections as independent fields, which we call the first-order formalism. Although such suggestions have been made previously in the context of gauge theories,[20] no concrete calculations exist to our knowledge. This may be because of ambiguities in interpretation and, therefore, a lack of a recipe for calculations.

Recently,[21] however, it was shown that first-order treatment of the simple $R + R^2$ action yields a conformally metric theory, which implies breakdown of the Einstein equivalence principle due to a breakdown of conformal symmetry. Since R^2 contributions are insignificant now, such a violation would not be observable at this time. At the time when curvature becomes significantly large, quadratic contributions will become important and a framework in which to include such contributions was developed. With the formalism of the $R + R^2$ gravity developed in the first-order regime, we will attempt to look at cosmology in four dimensions.

Although working with second-order equations is one reason to treat the metric and the connections independently, our motives here are more fundamental; namely, preserving generality. There are no *a priori* reasons to assume metric compatibility in the strong curvature epoch. Furthermore, there is no reason to assume the metric as the only independent field describing gravity at early times. In fact, one would hope that the relation between the metric and the connections would emerge from a more fundamental principle such as the principle of least action. There is no better example of this than GR itself where first-order variation of the action, yields metric compatibility automatically.

Therefore, we will show that in the case of $R - \alpha R^2$ gravity, the first-order formalism action can be rewritten in terms of the metric compatible fourth-order part plus contributions from the metric-incompatible part of the curvature. Fourth-order gravity can thus be thought of as a special case of the theory constructed in this manner namely, where the latter contribution vanishes. In general, however, the metric-incompatible part can modify the fourth-order theory significantly. We will show that in the case of cosmology there exists a solution without singularity at $t = 0$. Expectedly, the size of the universe at this time is of the order of the free parameter of the theory, α, introduced by the quadratic contribution.

One must also mention the work of Whitt[22] which seems to resolve the problem of dealing with fourth-order equations. This is done by solving, in a conformal space, the pure Einstein gravity coupled to a scalar field. However, we feel that there, also, generality has been lost due to the assumption of metric compatibility.

In the first part of this paper, we will start with the discussion of the field equations as derived in the two formalisms. We will show that requiring metric compatibility of the connections after the action has been varied with respect to the connections and the metric independently, leads to the recovery of the fourth-order equations. In the second part, we will apply the field equations derived and the method described in Ref. 21 to the classical Friedmann cosmology of

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a spherically symmetric ball of dust described by the Robertson–Walker metric. We will show how under certain assumptions the equations of cosmology evolve into the standard GR equations. The conventions used here are those of Weinberg.[23]

II. THE FIELD EQUATIONS

A detailed derivation of the first-order field equations can be found in Ref. 21. Here we give a short summary. Let us start with the simplest unitary action:

$$\mathcal{A} = \int \sqrt{-g}(R - \alpha R^2 + T_{\text{matter}})d^4x, \tag{2.1}$$

where $R = R_{\mu\nu}\, g^{\mu\nu}$. The Ricci tensor $R_{\mu\nu}$ is now a function of the connection field and its derivatives and its variation in a geodesic frame, neglecting torsion, can be written as

$$\delta R_{\mu\nu} = \nabla_\lambda(\delta\Gamma^\lambda{}_{\mu\nu}) - \nabla_\nu(\delta\Gamma^\lambda{}_{\mu\lambda}). \tag{2.2}$$

Assuming that T_{matter} is independent of the connections, varying the full action now with respect to the metric $g_{\mu\nu}$ and the connections $\Gamma^\lambda{}_{\mu\nu}$, respectively, gives

$$R_{\mu\nu} - \tfrac{1}{2} g_{\mu\nu}R - 2\alpha R(R_{\mu\nu} - \tfrac{1}{4} g_{\mu\nu}R) = -8\pi G T_{\mu\nu} \tag{2.3}$$

and

$$\nabla_\mu(\sqrt{-g}g^{\alpha\beta}(1 - 2\alpha R)) = 0. \tag{2.4}$$

Manipulating the last equation yields

$$\nabla_\alpha g_{\mu\nu} = b_\alpha g_{\mu\nu}, \tag{2.5}$$

where

$$b_\mu = 2\alpha R_{,\mu}/(1 - 2\alpha R). \tag{2.6}$$

The connections can then be derived, using Eq. (2.5) as

$$\Gamma^\lambda{}_{\mu\nu} = \tfrac{1}{2} g^{\lambda\delta}(g_{\delta\mu,\nu} + g_{\delta\nu,\mu} - g_{\mu\nu,\delta}) - \tfrac{1}{2}(\delta^\lambda{}_\mu b_\nu + \delta^\lambda{}_\nu b_\mu - g_{\mu\nu}b^\lambda). \tag{2.7}$$

The above two equations represent the main deviations from GR. The former exhibits violation of the Einstein equivalence principle (EEP) and the latter exhibits separation from metric compatibility by the additional contribution to the first term, the Christoffel connection. It should be noted that deviations are of order α which can be important only when αR^2 contributions are comparable to R. This is expected to occur around planck time.

In order to interpret the results in terms of the more familiar fourth-order gravity, one can rewrite all the geometric tensors in terms of their metric compatible counterparts plus contributions from the vector b_μ. In particular, we get

$$R_{\mu\nu} = R^{(0)}{}_{\mu\nu} - \tfrac{3}{2}D_\mu b_\nu + \tfrac{1}{2}D_\nu b_\mu - \tfrac{1}{2} g_{\mu\nu}D\cdot b - \tfrac{1}{2}b_\mu b_\nu + \tfrac{1}{2} g_{\mu\nu}b^2, \tag{2.8}$$

and

$$R = R^{(0)} - 3D\cdot b + \tfrac{3}{2} b^2. \tag{2.9}$$

Here, the superscript (0) denotes the metric-compatible quantities and D_μ is the corresponding covariant derivative. The inner products are with respect to the metric. Now, one can rewrite the original action, aside from the matter contribution as

$$A = \int \sqrt{-g}(\mathcal{L}_c + \mathcal{L}_{\text{nc}})d^4x, \tag{2.10}$$

where

$$\mathcal{L}_c = R^{(0)} - \alpha(R^{(0)})^2 \tag{2.11}$$

is the metric-compatible fourth-order action which is usually considered in higher-derivative gravity and

$$\mathcal{L}_{\text{nc}} = -3D\cdot b(1 - 2\alpha R^{(0)}) + \tfrac{3}{2}b^2(1 - 2\alpha R^{(0)}) - \alpha[9(D\cdot b)^2 + \tfrac{9}{4}b^4 - 9(D\cdot b)b^2]. \tag{2.12}$$

Thus $\mathcal{L}_{\text{nc}}$ represent the metric noncompatible addition that is ignored if one works with fourth-order action to begin with. This Lagrangian includes a massive vector field b_μ with couplings to itself and the curvature.

First-order formalism therefore provides a general treatment of quadratic gravity which is equivalent to a theory of fourth-order gravity coupled to a self-interacting massive vector field. In the limit where b_μ vanishes, the usual fourth-order theory is recovered. Furthermore, this procedure replaces the fourth-order field equations by two sets of second-order equations (2.3) and (2.4).

One might consider gauging away the b_μ field by a conformal transformation given by

$$g'_{\mu\nu} = \Omega(x)^2 g_{\mu\nu}, \tag{2.13}$$

and

$$b'_\lambda = b_\lambda + 2\Omega^{-1}\Omega_{,\lambda}. \tag{2.14}$$

However, if the energy-momentum tensor has a nonvanishing trace, b_μ is defined via Eq. (2.6), and the trace of Eq. (2.3):

$$R = 8\pi G T,$$

$$b_\mu = [16\alpha\pi G/(1 - 16\alpha\pi G T)]T_{,\mu}. \tag{2.15}$$

For conformally noninvariant matter, given the trace of the energy momentum tensor T, b_μ is fixed and cannot be gauged away.

III. FRIEDMANN COSMOLOGY

Having derived the necessary ingredients for calculations, we will now look at a practical aspect, namely cosmology. We assume spherical symmetry, homogeneity, and isotropy of the early universe presented by the Robertson–Walker metric:

$$ds^2 = -c^2 dt^2 + a(t)^2 \times\left(\frac{dr^2}{1 - Kr^2} + r^2 d\theta^2 + r^2 \sin^2\theta\, d\phi^2\right). \tag{3.1}$$

We will confine ourselves to the spatially flat ($K = 0$) case at this time. However, the upcoming arguments can easily be generalized to the $K = \pm 1$ cases. The energy momentum tensor is that of a perfect fluid:

$$T_{\mu\nu} = p g_{\mu\nu} + u_\mu u_\nu(p + \rho), \tag{3.2}$$

where p and ρ are the pressure and mass density, respectively. The conservation laws are given as in Ref. 21 by

$$\nabla_\mu[G^\mu{}_\nu/(1 - 16\pi G\alpha T)] = 0, \tag{3.3}$$

$G^\mu{}_\nu$ being the Einstein tensor, which interestingly yields

$$\frac{d}{dt}(\rho a^3) = -p\frac{d}{dt}(a^3). \tag{3.4}$$

The vector b_μ is now given by Eq. (2.13) and is a timelike vector. It is convenient to introduce the variable U defined as

$$U = 1 - 2\alpha R = 1 - 16\pi G\alpha(3p - \rho), \tag{3.5}$$

and assume an equation of state given by $p = (\gamma - 1)\rho$, which together with Eq. (3.4) gives

$$\rho = \rho_0(a_0/a(t))^{3\gamma}, \tag{3.6}$$

where ρ_0 and a_0 are constants.

The two independent equations of motion are then given by

$$3\frac{1}{a}\frac{d^2a}{dt^2} - \frac{3}{2}\frac{db_0}{dt} - \frac{3}{2}\frac{1}{a}\frac{da}{dt}b_0 = -\frac{8\pi G}{U}\left\{\rho - \frac{U^2-1}{64\pi G\alpha}\right\}, \tag{3.7}$$

$$-\frac{1}{a}\frac{d^2a}{dt^2} - 2\left(\frac{1}{a}\frac{da}{dt}\right)^2 + \left(\frac{5}{2}\frac{1}{a}\frac{da}{dt}b_0 + \frac{1}{2}\frac{db_0}{dt} - \frac{1}{2}(b_0)^2\right) = -\frac{8\pi G}{U}\left\{p + \frac{U^2-1}{64\pi G\alpha}\right\}. \tag{3.8}$$

Note that in the limit $\alpha \to 0$, $U \to 1$ the field equations reduce to those of GR. Using Eqs. (3.5) and (3.6), U can now be written in terms of $a(t)$ and its derivatives and, after some manipulations, one arrives at

$$\left(\frac{1}{a}\frac{da}{at}\right)^2 = \frac{8}{3}\pi G\rho\left(\frac{1 + (3\gamma/4)(1/U - 1)}{[1 + \frac{3}{2}\gamma(1/U - 1)]^2}\right), \tag{3.9}$$

where, now,

$$U = 1 - 16\pi G\alpha(3\gamma - 4)\rho_0(a_0/a(t))^{3\gamma}. \tag{3.10}$$

Equation (3.9), together with Eq. (3.10), can now be in principle solved.

It is interesting that GR limit is automatically satisfied as the expansion parameter $a(t)$ increases. This is a rather desirable property since we know that GR explains the present epoch successfully. We will examine the behavior of the solutions of Eq. (3.9) by considering a particle in an effective potential given by

$$V(a) = -\frac{8}{3}\pi G\rho(a)\left(\frac{1 + (3\gamma/4)(1/U(a) - 1)}{[1 + \frac{3}{2}\gamma(1/U(a) - 1)]^2}\right)a^2, \tag{3.11}$$

and total energy:

$$E = \left(\frac{da}{dt}\right)^2 + V(a) = 0. \tag{3.12}$$

The behavior of the soutions of Eq. (3.12) can be studied by analyzing the shape of the potential $V(a)$, as a function of parameter γ and the sign of α.

We plot $V(a)$ as a function of $a(t)$ for $0 < a(t) < \infty$. Ruling out $\gamma < 0$, there are four possible scenarios:

Case (i): $\alpha > 0$, $\gamma > 4/3$,

Case (ii): $\alpha > 0$, $0 < \gamma < 4/3$,

Case (iii): $\alpha < 0$, $\gamma < 4/3$,

Case (iv): $\alpha < 0$, $0 < \gamma < 4/3$.

The potential $V(a)$ has two possible zeros, at $U(a) = 0$ and $U(a) = U_1 = 3\gamma/(3\gamma - 4)$ corresponding to $a = \hat{a} = a_0(16\pi G\alpha(3\gamma - 4)\rho_0)^{1/3\gamma}$, and $a = \hat{a}_1 = a_0(-4\pi G\alpha \times (3\gamma - 4)^2\rho_0)^{1/3\gamma}$, respectively, as shown by Figs. 1–4. The total energy is given by the $E = 0$ axis and thus the physical solutions are those where $E > V(a)$. If desired, one can generalize to the $K = \pm 1$ by considering $E = \pm 1$ for the closed and open universe scenarios. Let us now study the behaviour of $a(t)$ in the above cases.

A. Case (i)

This is one of the most striking cases. The effective potential introduces a barrier in the first few time constants. The $t = 0$ singularity is therefore avoided. The wall crosses the $E = 0$ axis at $U = 0$, $a = \check{a}$. To see the behavior of $a(t)$ at this point, we note that Eq. (3.9), at $U \simeq 0$ can be written as

$$\left(\frac{1}{a}\frac{da}{dt}\right)^2 \simeq \frac{8}{3}\pi G\rho\frac{U}{3\gamma} = \frac{8}{9\tau}\pi G\rho_0\left(\frac{a_0}{a}\right)^{3\gamma} \times\left[1 - 16\pi G\alpha(3\gamma - 4)\rho_0\left(\frac{a_0}{a}\right)^{3\gamma}\right]. \tag{3.13}$$

The solution is found exactly:

$$a(t) = a_0(16\pi G\alpha(3\gamma - 4)\rho_0 + 2\pi G\gamma\rho_0 t^2)^{1/3\gamma}. \tag{3.14}$$

Thus at $t = 0$, $a = \check{a}$ and the parameter α determines the initial size at $t = 0$. One can show that the second derivative of $a(t)$ at $t = 0$ is positive and becomes negative at later times. Solving Eq. (3.9) numerically demonstrates this as shown in Fig. 5. The plot illustrates the evolution of $a(t)$ for $\gamma = 5/3$. At large t, the potential gradually increases and thus the expansion rate slows down as kinetic energy decreases.

B. Case (ii)

In this case, the potential $V(a)$ does not meet the $E = 0$ axis and stays in the negative region at all times. The $a = 0$ singularity resembles that of GR and the scenario is that of big-bang. The expansion slows down as kinetic energy decreases in later epochs.

C. Case (iii)

This is simillar to case *i*, except that the potential has its zero at $a = \check{a}_1$. Again, the potential barrier avoids the initial singularity.

D. Case (iv)

This is the only case where $V(a)$ has two physical zeros. The hump produced by the potential offers two classically

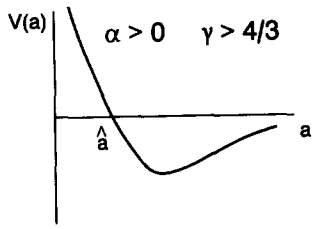

FIG. 1. Energy diagrams: The effective potential $V(a)$ is plotted against the expansion parameter a. The horizontal axis represents total energy $E = 0$.

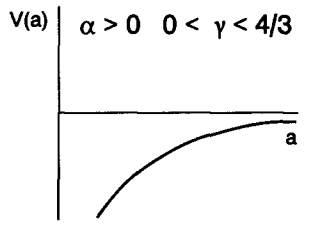

FIG. 2. Same as Fig. 1.

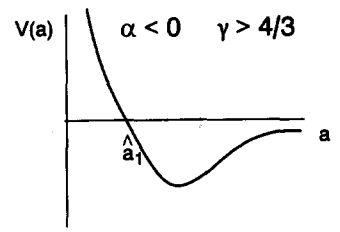

FIG. 3. Same as Fig. 1.

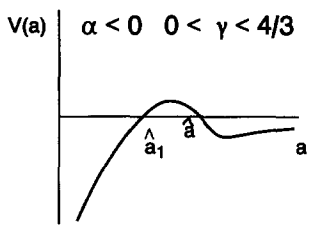

FIG. 4. Same as Fig. 1.

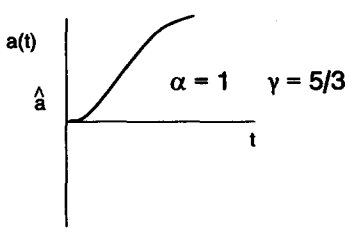

FIG. 5. Time evolution of the expansion parameter $a(t)$ for $\alpha = 1, \gamma = 5/3$.

distinct regions; a negatively unbound region between $a = 0$ and $a = \check{a}_1$ which results in a "big crunch," and a universe bouncing between $a = \check{a}$ and $a = \infty$.

Although the shape of the effective potential introduces new possibilities that may exist in the early times, one cannot take these effects too seriously. After all, we have said nothing of quantum effects themselves which are expected to be prominent at early stages. We must, therefore, emphasize the very speculative nature of this work and appreciate the results at their face value.

IV. CONCLUSIONS

We have used the prescription given for the first-order treatment of a gravitational action, composed of the Einstein term plus a quadratic in the scalar curvature, to discuss the classical properties of the implied field equations and to demonstrate a physical calculation where implications of this formalism can differ from the usual fourth-order results. The advantages and the results of taking this route are as follows.

(a) The formalism does not make the assumption of metric compatibility. One can envision a scenario where metric compatibility is a low-energy limit property of space time. The first-order treatment of the quadratic action is, therefore, an extension of the fourth-order gravity in generality.

(b) The field equations are only second order so the usual difficulties with fourth-order equations are bypassed. The difficulties, however, are replaced by the addition of a vector that is interpreted as a contribution of the stress-energy tensor to the connections.

(c) In the standard Friedmann scenarios, the long-time limit of the evolution equations yield metric compatibility and the standard cosmological models based on general relativity are recovered.

(d) One can find solutions in cosmology with no singularity at $t = 0$.

It would be interesting to study the Kaluza–Klein scenario. It is reasonable to hope that since singularity can be avoided under certain assumptions, one could stop the collapse of the extra dimensions by this procedure. Also, the study of the semiclassical approximation in this formalism is of interest. A natural question arises: Is metric compatibility a classical limit of a quantum theory of gravity? This is currently under consideration by the author.

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Shear-free perfect fluids in general relativity II. Aligned, Petrov type III space-times

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Petrov type III, shear-free, perfect fluid solutions of the Einstein field equations, with a barotropic equation of state $p = p(w)$ satisfying $w + p \neq 0$, are investigated. It is shown that if the acceleration of the fluid is orthogonal to the two-spaces spanned by the repeated principal null direction of the Weyl tensor and the fluid four-velocity, or if the fluid four-velocity lies in the two-spaces spanned by the principal null directions of the Weyl tensor, then the fluid's volume expansion is zero.

I. INTRODUCTION

There is now considerable evidence in the literature that supports the conjecture that general relativistic, shear-free perfect fluids which obey a barotropic equation of state $p = p(w)$ such that $w + p \neq 0$, are either nonexpanding or irrotational. For example, this conjecture is known to hold in (i) all dust space-times (Ellis[1]), (ii) conformally flat space-times (Ellis[2]), (iii) spatially homogeneous space-times (King and Ellis[3] and White[4]), (iv) shear-free radiation, $p = \frac{1}{3}w$ (Treciokas and Ellis[5]), (v) the case when the fluid vorticity ω_a and acceleration $\dot{u}_a$ are parallel (White and Collins[6]), and (vi) the case when the magnetic part of the Weyl tensor, with respect to the fluid flow, vanishes (Collins[7]). More recently, the conjecture has been shown to hold for type N space-times (Carminati[8]) and for the case when the fluid's expansion and energy density are assumed to be functionally dependent (Lang and Collins[9]), and thus includes hypersurface-homogeneous space times.

Shear-free fluids with a barotropic equation of state are of considerable interest in cosmology from both the theoretical and observational point of view[10] (Friedmann–Robertson–Walker models, Gödel solution, the spherically symmetric but spatially inhomogeneous Wyman solution, etc.). For example, certain observational aspects of shear-free fluids that are relevant to cosmology are most readily highlighted when one considers the formulas for recessional motion, relative red shift, and transverse motion of neighboring galaxies.[2] It then readily follows that shear-free fluid solutions would retain the desirable feature of isotropy of local motion but allow the galactic red shift to be anisotropic if $\dot{u}_a \neq 0$ (the relative measure of this anisotropy would be given by the ratio $3|\dot{u}_a|/\theta$, where $\theta \neq 0$ is the volume expansion). Consequently, there would be a preferred direction, which coincides with that of $\dot{u}_a$, as indicated by the maximum red shift. In addition, if the fluid is nonrotating, the transverse motion of neighboring galaxies has an isotropic evolution. On the theoretical side, the general validity of the conjecture together with the possibility that relativistic kinetic theory requires perfect fluids to be shear-free,[5] would impart a sense of uniqueness[11] to the Friedmann–Robertson–Walker cosmological models since it has been shown that they are the only physically reasonable space-times which represent an expanding, shear-free, irrotational perfect fluid, on a global scale.

Finally, it is interesting to note that there are Newtonian self-gravitating, shear-free fluids that are expanding and rotating.[2] Therefore, if the conjecture were to be generally valid, then it would be a result that would highlight certain essential differences between fluid dynamics in Newtonian theory and in general relativity.

This is the second in a series of papers dedicated to the study of the general validity of the above conjecture in algebraically special space-times. We shall show that for any shear-free, perfect fluid source with $p = p(w)$ and $w + p \neq 0$, of a type III space-time where either the acceleration of the fluid is orthogonal to the two-spaces spanned by the repeated principal null direction of the Weyl tensor and the fluid four-velocity, or the perfect fluid is aligned with the Weyl tensor, then the fluid's volume expansion is zero.

The plan of this article is as follows. Section II contains the main result in the form of a theorem. The proof is given in Sec. III, and Sec. IV contains some concluding remarks. This paper presupposes a knowledge of the Newman–Penrose (NP) formalism. All considerations will be local. We have chosen geometrized units so that $8\pi G = 1$, $c = 1$, where G is the Newtonian gravitational constant and c is the speed of light in vacuum. Our conventions for the Riemann and Ricci tensors and the signature of the space-time are those of NP.

II. THE MAIN RESULT

In this article, we shall be investigating Petrov type III, perfect fluid solutions of the Einstein field equations,[12]

$$R_{ab} - \tfrac{1}{2}Rg_{ab} = -T_{ab}, \tag{2.1}$$

where

$$T_{ab} = (w+p)u_a u_b - pg_{ab}, \quad u_a u^a = 1, \tag{2.2}$$

in which the fluid congruence is shear-free and the pressure satisfies a barotropic equation of state,

$$p = p(w). \tag{2.3}$$

Our main result is the following.

Theorem: Consider any Petrov type III, shear-free perfect fluid solution of the Einstein field equations, with a baro-

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tropic equation of state $p = p(w)$ satisfying $w + p \neq 0$. If the acceleration of the fluid is orthogonal to the two-spaces spanned by the repeated principal null direction of the Weyl tensor and the fluid four-velocity or if the fluid four-velocity lies in the two-spaces spanned by the principal null directions of the Weyl tensor, then the fluid volume expansion is zero.

III. PROOF OF THE THEOREM[13]

Let C_{abcd} and u_a denote the Weyl tensor and four velocity of the fluid, respectively. The assumption that C_{abcd} is of Petrov type III seems to naturally lead to the following specialization of the principal null tetrad $\{l,n,m,\bar{m}\}$. First, l is chosen to be the repeated principal null direction of the Weyl tensor so that

$$C_{abc[d}\, l_{e]} l^c = 0, \quad C_{abcd} l^d \neq 0. \tag{3.1}$$

Therefore the NP Weyl tensor components satisfy

$$\Psi_0 = \Psi_1 = \Psi_2 = 0, \quad \Psi_3 \neq 0. \tag{3.2}$$

Next, by a null rotation that leaves l fixed, it is possible to make n lie in the two-spaces spanned by l and u. Finally, by rescaling l and n it is then possible to achieve

$$u = 2^{-1/2}(l + n). \tag{3.3}$$

From Eqs. (2.1)–(2.2) and (3.3), it follows that the NP components of the trace-free Ricci tensor $S_{ab} \equiv R_{ab} - \frac{1}{4} R g_{ab}$ satisfy

$$\Phi_{01} = \Phi_{12} = \Phi_{02} = 0, \tag{3.4}$$

$$\Phi_{00} = \Phi_{22} = 2\Phi_{11} = \tfrac{1}{4}(w + p). \tag{3.5}$$

The Ricci scalar $R \equiv 24\Lambda$ is given by

$$R = w - 3p. \tag{3.6}$$

It should be noted that the tetrad is still not fixed uniquely. The remaining tetrad freedom is expressed by the rotation

$$\tilde{l}^a = l^a, \quad \tilde{n}^a = n^a, \quad \tilde{m}^a = e^{i\xi} m^a, \tag{3.7}$$

where ξ is a real function.

The shear tensor σ_{ab}, vorticity tensor ω_{ab}, and expansion θ of the fluid four-velocity (3.3) are given by[14]

$$\sigma_{ab} = A_1 (v_a v_b - m_{(a}\bar{m}_{b)}) + A_2 v_{(a} m_{b)} + \bar{A}_2 v_{(a}\bar{m}_{b)} + A_3 m_a m_b + \bar{A}_3 \bar{m}_a \bar{m}_b, \tag{3.8}$$

$$\omega_{ab} = B_1 v_{[a} m_{b]} + \bar{B}_1 v_{[a}\bar{m}_{b]} + B_2 m_{[a}\bar{m}_{b]}, \tag{3.9}$$

and

$$\theta = 2^{-1/2}(\epsilon + \bar{\epsilon} - \gamma - \bar{\gamma} - \rho - \bar{\rho} + \mu + \bar{\mu}), \tag{3.10}$$

where

$$A_1 = -\tfrac{1}{3} 2^{-1/2}\{\rho + \bar{\rho} - \mu - \bar{\mu} + 2(\epsilon + \bar{\epsilon}) - 2(\gamma + \bar{\gamma})\},$$

$$A_2 = -\tfrac{1}{2}\{\bar{\tau} + \pi + 2(\alpha + \bar{\beta}) - \bar{\kappa} - \nu\},$$

$$A_3 = 2^{-1/2}(\bar{\sigma} - \lambda),$$

$$B_1 = \tfrac{1}{2}\{\bar{\tau} + \pi - 2(\alpha + \bar{\beta}) - \bar{\kappa} - \nu\},$$

$$B_2 = -2^{-1/2}\{\rho - \bar{\rho} + \mu - \bar{\mu}\},$$

and

$$v_a = 2^{-1/2}(l_a - n_a).$$

Therefore, the fluid is shear-free if and only if

$$\rho + \bar{\rho} - \mu - \bar{\mu} + 2(\epsilon + \bar{\epsilon}) - 2(\gamma + \bar{\gamma}) = 0, \tag{3.11a}$$

$$\tau + \bar{\pi} + 2(\bar{\alpha} + \beta) - \kappa - \bar{\nu} = 0, \tag{3.11b}$$

$$\bar{\sigma} - \lambda = 0. \tag{3.11c}$$

Next, using Eqs. (3.2), (3.4)–(3.6), and (3.11), the NP form of the Bianchi identities, after some straightforward manipulations, reduce to the following equivalent set

$$(D + \Delta) w = 3(w + p)(\gamma + \bar{\gamma} - \epsilon - \bar{\epsilon}), \tag{3.12a}$$

$$\dot{p}(\Delta - D) w = (w + p)(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}), \tag{3.12b}$$

$$\delta w = 3(w + p)(\bar{\alpha} + \beta), \tag{3.12c}$$

$$\bar{\sigma} = \lambda = 0, \tag{3.12d}$$

$$\kappa = \bar{\pi} + (1 + 3\dot{p})(\bar{\alpha} + \beta), \tag{3.12e}$$

$$Dw = 12\kappa\Psi_3 + \tfrac{3}{2}(w + p)(\bar{\rho} - \mu), \tag{3.12f}$$

$$D\Psi_3 = 2(\rho - \epsilon)\Psi_3 - \kappa\Psi_4 + \tfrac{1}{2}(w + p)(\alpha + \bar{\beta}), \tag{3.12g}$$

$$\delta\Psi_3 = 2(\kappa + \tau - \beta)\Psi_3, \tag{3.12h}$$

$$D\Psi_4 - \bar{\delta}\Psi_3 = 2(\alpha + 2\pi)\Psi_3 + (\rho - 4\epsilon)\Psi_4, \tag{3.12i}$$

$$\delta\Psi_4 - \Delta\Psi_3 = 2(\gamma + 2\mu)\Psi_3 + (\tau - 4\beta)\Psi_4 + \tfrac{3}{2}(w + p)(\alpha + \bar{\beta}), \tag{3.12j}$$

where $\ll \cdot \gg$ denotes differentiation with respect to w.

Henceforth, we shall assume that $\dot{p}(1 - 3\dot{p}) \neq 0$, as the conjecture essentially has been proven in the cases when $\dot{p} = 0$ (Ellis[1]) and when $\dot{p} = \frac{1}{3}$ (Treciokas and Ellis[5]). Equations (3.11) and (3.12) imply

$$24\kappa\Psi_3 = (w + p)\{\tfrac{3}{2}(\rho - \bar{\rho} + \mu - \bar{\mu}) - (1/\dot{p})(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma})\}, \tag{3.13}$$

and

$$\tau = \bar{\nu} + (3\dot{p} - 1)(\bar{\alpha} + \beta). \tag{3.14}$$

Combining some of the NP Eqs. (4.2), together with Eqs. (3.11)–(3.12) yields

$$\delta(\rho - \bar{\mu}) = (\bar{\alpha} + \beta)[\bar{\rho} + \mu + 3\dot{p}(\rho - \bar{\rho} + \mu - \bar{\mu})] - \bar{\Psi}_3, \tag{3.15a}$$

$$D(\bar{\alpha} + \beta) - \delta(\epsilon + \bar{\epsilon}) = (\bar{\alpha} + \beta)(\bar{\rho} - 2\bar{\epsilon}) + \bar{\pi}(\bar{\rho} + \epsilon + \bar{\epsilon}) - \kappa(\mu + \gamma + \bar{\gamma}), \tag{3.15b}$$

and

$$\delta(\gamma + \bar{\gamma}) - \Delta(\bar{\alpha} + \beta) = -\bar{\nu}(\bar{\rho} + \epsilon + \bar{\epsilon}) + (\bar{\alpha} + \beta)(\mu - 2\gamma) + \tau(\mu + \gamma + \bar{\gamma}) + \bar{\Psi}_3. \tag{3.15c}$$

Applying the commutator $[\delta, \Delta + D]$ to w yields

$$\delta(\bar{\rho} - \mu) - 2(\Delta + D)(\bar{\alpha} + \beta) = (2/3\dot{p})(\tau + \bar{\pi})(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}) + 6\dot{p}(\bar{\alpha} + \beta)(\gamma + \bar{\gamma} - \epsilon - \bar{\epsilon}) + (\bar{\alpha} + \beta) \times [\mu - 2\gamma + 2\bar{\gamma} - 3\bar{\rho} - 2\epsilon + 2\bar{\epsilon} - 3\dot{p}(\rho - \bar{\rho} + \mu - \bar{\mu})] + \bar{\Psi}_3, \tag{3.16}$$

where use has been made of Eqs. (3.11), (3.12), and (3.15). Similarly, consideration of $[\delta, \Delta - D]w$ leads to

$$2(\Delta + D)(\bar{\alpha} + \beta) = (\tau + \bar{\pi})(\bar{\rho} - \rho + \bar{\mu} - \mu) + 2(\bar{\alpha} + \beta) \times [\bar{\rho} - \mu + 2\gamma - 2\bar{\epsilon} + 3\dot{p}(\epsilon + \bar{\epsilon} - \gamma - \bar{\gamma})]. \tag{3.17}$$

Equations (3.16) and (3.17) imply

$$\delta(\bar{\rho} - \mu) = (\tau + \bar{\pi})[(2/3\dot{p})(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}) + \bar{\rho} - \rho + \bar{\mu} - \mu] + (\bar{\alpha} + \beta)[\rho - \bar{\mu} - 2\mu - 3\dot{p}(\rho - \bar{\rho} + \mu - \bar{\mu})] + \bar{\Psi}_3. \tag{3.18}$$

Applying δ to Eq. (3.11b) yields

$$\delta(\bar{\alpha} + \beta) = (\bar{\alpha} + \beta)(\bar{\alpha} + 3\beta + 2\tau - 2\bar{\nu}) + \tfrac{1}{2}\bar{\Psi}_4, \tag{3.19}$$

so that δ may now be applied to Eq. (3.12e) with the result that

$$2(\bar{\alpha} + \beta)^2[(1 + 3\dot{p})(3\dot{p} - 1) + 9\ddot{p}(w + p)] + \bar{\Psi}_4(1 + 3\dot{p}) = 0. \tag{3.20}$$

Next, applying δ to Eq. (3.13) with subsequent use of Eqs. (3.12c), (3.14), (3.15), (3.17), and (3.18) leads to the important relation

$$\bar{\Psi}_3(1 + 3\dot{p}) - (\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}) \times [2\tau + (3\ddot{p}/\dot{p})(w + p)(\bar{\alpha} + \beta)] + \tfrac{1}{2}[\rho - \bar{\rho} + \mu - \bar{\mu}] \times [\bar{\nu}(1 + 3\dot{p}) + \tau(3\dot{p} - 1)] = 0. \tag{3.21}$$

By applying the commutator $[\bar{\delta}, \delta]$ to w, we obtain

$$(1/\dot{p})(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma})(\rho - \bar{\rho} + \bar{\mu} - \mu) + 3(\bar{\rho} - \rho + \bar{\mu} - \mu)(\mu + \bar{\mu} + \epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}) = 0, \tag{3.22}$$

where use has been made of NP Eqs. (4.2) and Eqs. (3.12). Combining Eqs. (3.13), (3.21), and (3.22) yields

$$(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma})\{(1/2\dot{p})[\rho - \bar{\rho} + \bar{\mu} - \mu][\bar{\kappa}\bar{\nu}(1 + 3\dot{p}) + \bar{\kappa}\tau(3\dot{p} - 1) - \tfrac{1}{8}(w + p)(1 + 3\dot{p})] - (3/\dot{p})[\mu + \bar{\mu} + \epsilon + \bar{\epsilon} + \gamma + \bar{\gamma}] \times [2\dot{p}\bar{\kappa}\tau + \tfrac{1}{24}(w + p) \times (1 + 3\dot{p}) + 3\ddot{p}(w + p)\bar{\kappa}(\bar{\alpha} + \beta)]\} = 0. \tag{3.23}$$

Thus we are naturally led to distinguish two separate cases: (a) $\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma} = 0$ and (b) $\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma} \neq 0$. Since the acceleration vector[14] $\dot{u}_a$ is given by

$$\dot{u}_a = 2^{-1/2}(\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma})v_a + \tfrac{1}{2}(\pi - \bar{\tau} - \bar{\kappa} + \nu)m_a + \tfrac{1}{2}(\bar{\pi} - \tau - \kappa + \bar{\nu})\bar{m}_a, \tag{3.24}$$

it follows that the condition $\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma} = 0$ can be interpreted geometrically as the requirement that the acceleration vector lie in the two-spaces spanned by m and $\bar{m}$; i.e.,

$$\dot{u}_{[a} m_b \bar{m}_{c]} = 0. \tag{3.24'}$$

We begin the proof of the first part of the Theorem by assuming

$$\epsilon + \bar{\epsilon} + \gamma + \bar{\gamma} = 0. \tag{3.25}$$

From Eq. (3.22), we immediately find that either

$$\mu + \bar{\mu} = 0, \tag{3.26}$$

or if $\mu + \bar{\mu} \neq 0$, then

$$\rho - \bar{\rho} + \mu - \bar{\mu} = 0. \tag{3.27}$$

Case I: $\mu + \bar{\mu} = 0$.

It follows from Eqs. (3.13) and (3.21) that either

$$\bar{\rho} - \rho - 2\mu = 0, \tag{3.28}$$

or if $\bar{\rho} - \rho - 2\mu \neq 0$, then

$$(1 + 3\dot{p})(w + p) - 8\bar{\kappa}\Big(\bar{\nu}[1 + 3\dot{p}] + \tau[3\dot{p} - 1]\Big) = 0. \tag{3.29}$$

Case IA: $\bar{\rho} - \rho - 2\mu = 0$.

Then, by Eq. (3.21), it follows that

$$1 + 3\dot{p} = 0. \tag{3.30}$$

Equations (3.12e) and (3.13) immediately yield

$$\kappa = \pi = 0, \tag{3.31}$$

while Eq. (3.11a) leads to

$$2(\gamma + \bar{\gamma}) = \bar{\rho} - \mu = \rho - \bar{\mu} = (\rho + \bar{\rho})/2. \tag{3.32}$$

Applying the operator D to Eq. (3.26) and using Eqs. (3.31), (3.32) with NP Eqs. (4.2), we obtain

$$\mu^2 + 2\Lambda = 0. \tag{3.33}$$

Again, we apply D to Eq. (3.33) with the consequence that

$$(\epsilon + \bar{\epsilon})(w + p - 24\Lambda) = 0, \tag{3.34}$$

and, therefore, because of (3.30), $\epsilon + \bar{\epsilon} = 0$ since $\dot{p} \neq 0$. Thus $\gamma + \bar{\gamma} = \bar{\rho} - \mu = \rho - \bar{\mu} = \rho + \bar{\rho} = 0$, and it follows that the fluid has zero volume expansion; i.e. $\theta = 0$.

Case IB: $\bar{\rho} - \rho - 2\mu \neq 0$.

The commutators $[\Delta, D]$, $[\delta, \Delta - D]$ and $[\delta, D]$ applied to w yield

$$(D - \Delta)(\gamma + \bar{\gamma}) = (\tau + \bar{\pi})(\alpha + \bar{\beta}) + (\bar{\tau} + \pi)(\bar{\alpha} + \beta), \tag{3.35}$$

$$(D - \Delta)(\bar{\alpha} + \beta) = (\bar{\alpha} + \beta)(\bar{\rho} + \mu + \epsilon - \bar{\epsilon} - 5\gamma - 3\bar{\gamma}), \tag{3.36}$$

and

$$\delta(\gamma + \bar{\gamma}) - D(\bar{\alpha} + \beta) = (\bar{\alpha} + \beta)[(2 + 3\dot{p})(\gamma + \bar{\gamma}) - \bar{\rho} - \epsilon + \bar{\epsilon}], \tag{3.37}$$

respectively, where use has been made of Eqs. (3.11), (3.12), and NP (4.2).

Combining Eqs. (3.37) and (3.15b), we obtain

$$2\delta(\gamma + \bar{\gamma}) = 3(1 + \dot{p})(\bar{\alpha} + \beta)(\gamma + \bar{\gamma}) + \bar{\pi}(\bar{\rho} - \gamma - \bar{\gamma}) - \kappa(\mu + \gamma + \bar{\gamma}), \tag{3.38}$$

while Eqs. (3.15b), (3.15c), and (3.36) imply

$$2\bar{\Psi}_3 = \bar{\nu}(\bar{\rho} - \rho) - 2\tau\mu, \tag{3.39}$$

where, in addition, use has been made of Eq. (3.14), together with Eq. (3.11a) which in this case reduces to

$$\rho + \bar{\rho} = 4(\gamma + \bar{\gamma}). \tag{3.40}$$

To proceed further we need to distinguish whether or not $(\bar{\alpha} + \beta)(1 + 3\dot{p})$ is zero.

Case IB(i): $(\bar{\alpha}+\beta)(1+3\dot{p})\neq 0$.

Rewriting Eq. (3.19) using (3.20), yields the following useful form

$$\delta(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)[\bar{\alpha}+3\beta-2\bar{\nu}+2\tau+H(\bar{\alpha}+\beta)], \tag{3.41}$$

where

$$H\equiv[(1+3\dot{p})(1-3\dot{p})-9\ddot{p}(w+p)]/(1+3\dot{p}). \tag{3.42}$$

We may now apply the commutator $[\delta,\Delta-D]$ to $\bar{\alpha}+\beta$, which, after a lengthy computation, leads to

$$4(H+9\dot{p}-3)(\bar{\alpha}+\beta)(\gamma+\bar{\gamma}) + 4\mu(\bar{\alpha}+\beta)+\tau(\bar{\rho}-\rho)-2\mu\bar{\nu}=0, \tag{3.43}$$

since $(1+3\dot{p})(\bar{\alpha}+\beta)\neq 0$.

Next, using Eq. (3.21), which in this case reduces to

$$2\bar{\Psi}_3(1+3\dot{p})+(\rho-\bar{\rho}+2\mu) \times[\bar{\nu}(1+3\dot{p})+\tau(3\dot{p}-1)]=0, \tag{3.44}$$

together with Eqs. (3.13), (3.14), and (3.39), we obtain

$$4\mu(\bar{\alpha}+\beta)+\tau(\bar{\rho}-\rho)-2\mu\bar{\nu}=0, \tag{3.45}$$

and thus Eq. (3.43) reduces to

$$(H+9\dot{p}-3)(\gamma+\bar{\gamma})=0. \tag{3.46}$$

Equation (3.45) may be equivalently expressed as

$$\kappa\tau\Psi_3+\mu(\bar{\alpha}+\beta)Q=0, \tag{3.47}$$

where

$$Q\equiv-(1+3\dot{p})(w+p)/8 = -\bar{\kappa}[\bar{\nu}(1+3\dot{p})+\tau(3\dot{p}-1)].$$

Applying the δ operator to Eq. (3.47) leads to

$$\mu(\bar{\alpha}+\beta)Q\left(H[\bar{\alpha}+\beta]-2\kappa-2\bar{\nu}-\bar{\pi}\right)-\kappa^2\bar{\nu}\Psi_3 + Q(\bar{\alpha}+\beta)\bar{\Psi}_3+3\mu(\bar{\alpha}+\beta)^2(w+p)\dot{Q}=0. \tag{3.48}$$

Case IB(ia): $\gamma+\bar{\gamma}\neq 0\Leftrightarrow\rho+\bar{\rho}\neq 0$.

We shall prove that this case is impossible. With the assumption that $\gamma+\bar{\gamma}\neq 0$, it follows from Eq. (3.46) that

$$H=3(1-3\dot{p}). \tag{3.49}$$

We now note that $\mu(\bar{\alpha}+\beta)Q\neq 0$. This is shown as follows: If $\mu Q=0$, then from (3.47) $\kappa\tau=0$ and hence because of Eq. (3.13), we must have $\tau=0$. It then follows from NP Eqs. (4.2) that $\bar{\nu}=0$, since $\kappa\neq 0$. However, $\tau=\bar{\nu}=0$ is impossible since we have assumed $(\bar{\alpha}+\beta)(3\dot{p}-1)\neq 0$. Equation (3.49) yields

$$\dot{Q}/Q=(9\dot{p}+1)/3(w+p). \tag{3.50}$$

Multiplying Eq. (3.48) by τ and then using Eqs. (3.47) and (3.50) leads to

$$(\tau+\bar{\pi})(\bar{\nu}-3\tau)=0, \tag{3.51}$$

since $\mu(\bar{\alpha}+\beta)Q\neq 0$. Suppose $\bar{\nu}=3\tau$. Then, Eq. (3.14) becomes $2\tau=(\bar{\alpha}+\beta)(1-3\dot{p})$, whereas NP Eqs. (4.2) yield $\bar{\Psi}_4=3\tau(2\bar{\alpha}+2\beta+\bar{\pi}-3\kappa)$. Combining these equations with Eq. (3.20) gives $\bar{\pi}=3\kappa+2(\bar{\alpha}+\beta)$, since $\tau\neq 0$, and it follows from (3.12e) that $2\kappa=-3(\bar{\alpha}+\beta)(1+\dot{p})$. Applying the δ operator to this equation leads to $3\ddot{p}(w+p)-2(1+\dot{p})(1+3\dot{p})=0$. However, Eq. (3.49) reads $9\ddot{p}(w+p)+2(1+3\dot{p})(1-3\dot{p})=0$. Comparison of these two equations immediately yields $1+3\dot{p}=0$, which is a contradiction, and, therefore, the subcase $\bar{\nu}=3\tau$ is impossible.

Next, suppose $\bar{\nu}\neq 3\tau$, then $\tau+\bar{\pi}=0$. In this case, the commutator $[\delta,\Delta-D]$ applied to $\rho+\bar{\rho}$ leads to $\rho+\bar{\rho}=4(\bar{\alpha}+\beta)$, since $(\rho+\bar{\rho})(\bar{\alpha}+\beta)\neq 0$. Finally, applying the operator $\Delta-D$ to this equation yields $\bar{\rho}+\mu+\epsilon-\bar{\epsilon}-5\gamma-3\bar{\gamma}=0$. The real part of this condition is $\rho+\bar{\rho}=8(\gamma+\bar{\gamma})$, which, together with Eq. (3.40), gives $\rho+\bar{\rho}=\gamma+\bar{\gamma}=0$, which contradicts our original assumption.

Case IB(ib): $\gamma+\bar{\gamma}=0$.

For this case, $\rho+\bar{\rho}=\gamma+\bar{\gamma}=\epsilon+\bar{\epsilon}=0$ and, therefore, $\theta=0$.

Case IB(ii): $(\bar{\alpha}+\beta)=0$, $(1+3\dot{p})\neq 0$.

From the NP Eq. (4.21), it follows that $\epsilon+\bar{\epsilon}=0$ and, consequently, $\rho+\bar{\rho}=\gamma+\bar{\gamma}=0$. From Eqs. (3.12e) and (3.15b), we obtain $\kappa(\bar{\rho}-\mu)=0$. Since $\bar{\rho}-\rho-2\mu\neq 0\Leftrightarrow\bar{\rho}\neq\mu$, it follows that $\kappa=0$. But, Eq. (3.13) then yields $\mu-\bar{\rho}=0$, which is a contradiction. Thus this case is impossible.

Case IB(iii): $1+3\dot{p}=0$.

From Eqs. (3.12e), (3.29), and NP Eqs. (4.2), we find that $\kappa-\bar{\pi}=\tau=\bar{\nu}=\bar{\alpha}+\beta=0$, since $\kappa\neq 0$. Next, the commutator $[\delta,D]$ applied to w together with the preceding conditions leads to $\delta(\gamma+\bar{\gamma})=\bar{\Psi}_3=0$, which contradicts the assumption of Petrov type III.

Case II: $\mu+\bar{\mu}\neq 0, \rho-\bar{\rho}+\mu-\bar{\mu}=0$.

For this case Eqs. (3.12e), (3.13), and (3.21) immediately yield

$$\kappa=\bar{\pi}=1+3\dot{p}=0, \tag{3.52}$$

and the commutators $[\delta,\Delta+D]$ and $[\delta,\Delta-D]$ applied to w lead to

$$D(\bar{\alpha}+\beta)=\tau\left(\frac{\rho}{2}-\frac{\bar{\mu}}{2}+\epsilon+\bar{\epsilon}\right) -(\bar{\alpha}+\beta)(\epsilon+3\bar{\epsilon})+\frac{\bar{\Psi}_3}{2}, \tag{3.53}$$

and

$$\Delta(\bar{\alpha}+\beta)=\tau(\bar{\mu}/2-\rho/2-\epsilon-\bar{\epsilon})+(\bar{\alpha}+\beta) \times(\bar{\mu}-\rho+5\gamma+3\bar{\gamma}-2\epsilon-2\bar{\epsilon})-\bar{\Psi}_3/2. \tag{3.54}$$

Equation (3.11a) reduces to

$$\rho-\bar{\mu}+2(\epsilon+\bar{\epsilon})=0. \tag{3.55}$$

Using Eqs. (3.53)–(3.55) together with NP Eqs. (4.2), the δ operator applied to Eq. (3.25) gives

$$\bar{\Psi}_3=2\mu(\bar{\alpha}+\beta). \tag{3.56}$$

Applying the D operator to this equation yields $(\bar{\alpha}+\beta)(w+3p)=0$, and, consequently,

$$w+3p=0, \tag{3.57}$$

which is consistent with $1+3\dot{p}=0$. Next, the commutator $[\delta,D]$ applied to Ψ_3 results in

$$\delta(\alpha+\bar{\beta})=(\alpha+\bar{\beta})(2\tau-3\beta-\bar{\alpha}). \tag{3.58}$$

This equation may be combined with NP Eq. (4.21) to give

$$\bar{\tau}(\bar{\alpha}+\beta)=\tau(\alpha+\bar{\beta}). \tag{3.59}$$

It will now prove convenient to consider the cases $\tau\neq 0$ and $\tau=0$ separately.

Case IIA: $\tau\neq 0$.

We shall show that this case is impossible. If δ is applied to the complex conjugate of Eq. (3.56), it follows that $\tau(\mu-\bar{\mu})(\alpha+\bar{\beta})=0$ and, therefore,

$$\rho=\bar{\rho},\quad \mu=\bar{\mu}. \tag{3.60}$$

Next, consideration of δ applied to Eq. (3.56) and the commutator $[\delta,\Delta]$ applied to $\bar{\alpha}+\beta$, in conjunction with various above equations, leads to

$$D\bar{\Psi}_4=2\bar{\Psi}_4(\mu-\epsilon-3\bar{\epsilon}), \tag{3.61}$$

and

$$\Delta\bar{\Psi}_4=8\mu\tau(\bar{\alpha}+\beta)-48(\bar{\alpha}+\beta)^2(\epsilon+\bar{\epsilon})-2\bar{\Psi}_4(\mu+2\bar{\gamma}+3\epsilon+3\bar{\epsilon}). \tag{3.62}$$

Equations (3.12i) and (3.61) imply

$$\bar{\delta}\Psi_3=-2\alpha\Psi_3+\Psi_4(2\mu-\rho-2\epsilon-2\bar{\epsilon}). \tag{3.63}$$

Applying the commutator $[\delta,\Delta]$ to $\alpha+\bar{\beta}$ yields

$$\Delta\tau=\tau(\epsilon+\bar{\epsilon}-2\bar{\gamma}-\mu)-8(\epsilon+\bar{\epsilon})(\bar{\alpha}+\beta),$$

and, consequently, we may now apply $[\delta,\Delta]$ to τ, from which it follows that

$$\bar{\Psi}_4(\epsilon+\bar{\epsilon})=\tau[(\epsilon+\bar{\epsilon})(5\bar{\alpha}+5\beta-2\tau)+\mu\tau] \tag{3.64}$$

We note that the case $\epsilon+\bar{\epsilon}=0$ is impossible since it would then follow that $\mu=0$. Applying $[\Delta,D]$ to τ yields

$$\Delta(\rho+\mu-\epsilon-\bar{\epsilon})+\rho(\mu+\epsilon+\bar{\epsilon})-(\epsilon+\bar{\epsilon})^2+2\bar{\tau}(\bar{\alpha}+\beta)+\mu(\mu-\epsilon-\bar{\epsilon})+2\tau\bar{\tau}+w/3=0, \tag{3.65}$$

whereas consideration of $[\Delta,D](\bar{\alpha}+\beta)$ leads to

$$(\bar{\alpha}+\beta)[\Delta(\rho+\mu)+\mu(2\rho+3\mu-5\epsilon-5\bar{\epsilon})+4\tau\bar{\tau}-3\rho^2-5\rho(\epsilon+\bar{\epsilon})-4\bar{\tau}(\bar{\alpha}+\beta)+w/3]+\bar{\tau}\bar{\Psi}_4=0, \tag{3.66}$$

where various above equations and NP Eqs. (4.2) have been used. Combining Eqs. (3.65) and (3.66) yields

$$(\bar{\alpha}+\beta)[\Delta(\epsilon+\bar{\epsilon})+(\epsilon+\bar{\epsilon})^2+\bar{\tau}(2\tau-6\bar{\alpha}-6\beta)]+\bar{\tau}\bar{\Psi}_4=0. \tag{3.67}$$

The operator D applied to Eqs. (3.55) and (3.64) leads to

$$w=6\mu(2\epsilon+2\bar{\epsilon}-\mu), \tag{3.68}$$

and

$$D(\epsilon+\bar{\epsilon})+(\epsilon+\bar{\epsilon})^2=0, \tag{3.69}$$

respectively. Equations (3.67) and (3.69) may now be compared with NP Eq. (4.2f), and, as a consequence, we find

$$(\epsilon+\bar{\epsilon})(8[\bar{\alpha}+\beta]^2-7\tau[\bar{\alpha}+\beta]+2\tau^2)-\tau^2\mu=0, \tag{3.70}$$

where use has been made of Eqs. (3.59), (3.64), and (3.68), and certain nonzero factors have been canceled throughout. Eliminating ρ from Eq. (3.65) by using Eq. (3.55), and then combining Eqs. (3.69) and NP (4.2f), eventually yields

$$\Delta\mu+\mu(\epsilon+\bar{\epsilon})+4\bar{\tau}(\bar{\alpha}+\beta)+\tau\bar{\tau}=0.$$

We may now apply $[\Delta,D]$ to μ which with subsequent use of various above equations and NP Eqs. (4.2) leads to

$$3\Delta(\epsilon+\bar{\epsilon})+3(\epsilon+\bar{\epsilon})^2-2\bar{\tau}(\bar{\alpha}+\beta)=0.$$

Finally, if we compare this equation with Eq. (3.67), and use Eqs. (3.64) and (3.70), we obtain $(\bar{\alpha}+\beta)(\epsilon+\bar{\epsilon})=0$, which is a contradiction.

Case IIB: $\tau=0$.

In this case, we have

$$\bar{\nu}=2(\bar{\alpha}+\beta). \tag{3.71}$$

The NP Eqs. (4.2) and Eq. (3.53) imply

$$\delta(\epsilon+\bar{\epsilon})=(\bar{\alpha}+\beta)(-\bar{\rho}-\epsilon-\bar{\epsilon})+\bar{\Psi}_3/2. \tag{3.72}$$

Next, the application of the operator Δ to Eq. (3.71) yields

$$\Delta\nu=2(\alpha+\bar{\beta})(2\bar{\gamma}-3\epsilon-3\bar{\epsilon}-\bar{\mu}), \tag{3.73}$$

where use has been made of Eqs. (3.54) and (3.55). Applying the commutator $[\Delta,D]$ to ν leads to, in conjunction with various above equations and NP Eqs. (4.2),

$$D(\epsilon+\bar{\epsilon})=\Delta(\epsilon+\bar{\epsilon})=-(\epsilon+\bar{\epsilon})^2, \tag{3.74}$$

where a common factor of $\bar{\alpha}+\beta\neq 0$ has been cancelled throughout. Also, using NP Eq. (4.2n) together with Eqs. (3.58) and (3.71), we find

$$\delta\nu=-2(\alpha+\bar{\beta})(\bar{\alpha}+3\beta), \tag{3.75}$$

and

$$\Delta\mu=\mu(\epsilon+\bar{\epsilon}-\mu)-w/6. \tag{3.76}$$

The operator Δ applied to Eq. (3.56) gives

$$\Delta\bar{\Psi}_3=-4(\bar{\alpha}+\beta)(\mu[\mu+\bar{\gamma}+2\epsilon+2\bar{\epsilon}]+w/12). \tag{3.77}$$

Finally, applying the commutator $[\delta,\Delta]$ to Ψ_3 and using Eqs. (3.12), (3.55), (3.56), (3.58), (3.71), (3.72), (3.77), and NP Eqs. (4.2m) and (4.2o) yields, after a lengthy computation, $\bar{\mu}(\alpha+\bar{\beta})(\bar{\alpha}+\beta)(\epsilon+\bar{\epsilon})=0$ and, consequently, $\epsilon+\bar{\epsilon}=0$, since μ and $\bar{\alpha}+\beta$ are nonzero. Thus we conclude from Eq. (3.10) that $\theta=0$ and the first part of the theorem is established; i.e., $\dot{u}_{[a}m_b\bar{m}_{c]}=0\Rightarrow\theta=0$.

We begin the proof of the second part of the theorem by assuming

$$\Psi_4=0, \tag{3.78}$$

which states that n is the second principal null direction of the Weyl tensor, so that, necessarily, the fluid four-velocity lies in the two-spaces spanned by the principal null directions of the Weyl tensor. From Eq. (3.20), it follows that either

$$\bar{\alpha}+\beta=0, \tag{3.79}$$

or if $\bar{\alpha}+\beta\neq 0$, then

$$9\dot{p}(w+p)+(1+3\dot{p})(3\dot{p}-1)=0. \tag{3.80}$$

Case I: $(\bar{\alpha}+\beta)(1+3\dot{p})\neq 0$.

Using Eqs. (3.11), (3.12), (3.16), (3.17), (3.19), (3.78), (3.80), and NP Eqs. (4.2), we may apply the operator δ to Eq. (3.21), from which it follows that, after a very lengthy calculation in which the nonzero factor $\dot{p}^2(1+\dot{p})$ was canceled throughout,

$$T_1T_2T_3=0, \tag{3.81}$$

where

$$T_1 \equiv 3\dot{p}(\bar{\mu}-\rho)+(1-3\dot{p})(\epsilon+\bar{\epsilon})+(1+3\dot{p})(\gamma+\bar{\gamma}),$$

$$T_2 \equiv \bar{\pi}+\bar{\nu}+(3\dot{p}-1)(\bar{\alpha}+\beta),$$

$$T_3 \equiv 24\dot{p}\bar{\nu}+5(3\dot{p}-1)^2(\bar{\alpha}+\beta).$$

Case IA: $T_1 = 0$.

We shall show that this case is impossible. For this case, we have

$$3\dot{p}(\bar{\mu}-\rho)+(1-3\dot{p})(\epsilon+\bar{\epsilon})+(1+3\dot{p})(\gamma+\bar{\gamma})=0, \tag{3.82}$$

which implies

$$\rho-\bar{\rho}+\mu-\bar{\mu}=0. \tag{3.83}$$

Substituting Eq. (3.83) into Eq. (3.22) yields

$$(\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma})(\rho-\bar{\rho})=0. \tag{3.84}$$

The case when $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$ is impossible since it then follows from Eq. (3.82) that $\rho-\bar{\mu}=2(\gamma+\bar{\gamma})=-2(\epsilon+\bar{\epsilon})$. Combining this result with Eq. (3.21) immediately gives $\bar{\Psi}_3(1+3\dot{p})=0$, which contradicts our original assumptions. Next, assume $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}\neq 0$. Then, $\rho=\bar{\rho}$, which implies $\mu=\bar{\mu}$. Therefore, Eq. (3.11a) reduces to $\rho-\mu+\epsilon+\bar{\epsilon}-\gamma-\bar{\gamma}=0$. Substituting this result into Eq. (3.82) yields $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$ which is a contradiction.

Case IB: $T_2 = 0$.

For this case, we have

$$\bar{\nu}=(1-3\dot{p})(\bar{\alpha}+\beta)-\bar{\pi}, \tag{3.85}$$

and, consequently,

$$\tau+\bar{\pi}=0. \tag{3.86}$$

Next, we consider the commutator $[\delta,\Delta-D]$ applied to $\bar{\alpha}+\beta$. After a very lengthy computation, we find that

$$\epsilon+\bar{\epsilon}=\gamma+\bar{\gamma}, \tag{3.87}$$

where Eqs. (3.11), (3.12), (3.16), (3.17), (3.19), (3.21), (3.78), (3.80), (3.85), and NP Eqs. (4.2) have been used, and the nonzero factor $\dot{p}(1-9\dot{p}^2)$ has been canceled throughout. Equations (3.11a) and (3.87) immediately yield $\rho+\bar{\rho}=\mu+\bar{\mu}$ and it follows that $\theta=0$.

Case IC: $T_3 = 0$.

We now require that

$$24\dot{p}\bar{\nu}+5(3\dot{p}-1)^2(\bar{\alpha}+\beta)=0. \tag{3.88}$$

Applying δ to Eq. (3.88) and using Eqs. (3.12), (3.14), (3.80), and NP Eqs. (4.2) leads to $8\dot{p}\bar{\pi}+(5\dot{p}+1)(3\dot{p}-1)(\bar{\alpha}+\beta)=0$. Similarly, again applying δ to this equation yields $(\bar{\alpha}+\beta)(3\dot{p}-1)^2/\dot{p}=0$ which is a contradiction. Thus this case is impossible.

Case II: $\bar{\alpha}+\beta\neq 0$, $1+3\dot{p}=0$.

Equation (3.21) yields

$$\tau(\rho-\bar{\rho}+\mu-\bar{\mu}+2\epsilon+2\bar{\epsilon}+2\gamma+2\bar{\gamma})=0. \tag{3.89}$$

Now, if $\tau\neq 0$, then $\rho-\bar{\rho}+\mu-\bar{\mu}=0$ and $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$, and consequently since this subcase is covered by the first part of the theorem, it follows that $\theta=0$. Next, we assume $\tau=0$. From Eqs. (3.12e) and (3.14), we have $\kappa=\bar{\pi}$, $\bar{\nu}=2(\bar{\alpha}+\beta)$, and from NP Eq. (4.2p) we find that $\kappa\bar{\nu}=0$. Since $\bar{\alpha}+\beta\neq 0$, then $\kappa=\bar{\pi}=0$, which, together with Eq. (3.13), yields $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$ and the conclusion that $\theta=0$ follows.

Case III: $\bar{\alpha}+\beta=0$.

In this case,

$$\kappa=\bar{\pi},\quad \tau=\bar{\nu}, \tag{3.90}$$

and it follows from NP Eqs. (4.2c) and (4.2i) that

$$\bar{\Psi}_3=(\rho-\bar{\mu})(\bar{\nu}+\bar{\pi})+2\bar{\nu}(\epsilon+\bar{\epsilon})-2\bar{\pi}(\gamma+\bar{\gamma}). \tag{3.91}$$

From NP Eq. (4.2l), we obtain

$$\rho\mu-\bar{\rho}\bar{\mu}+(\rho-\bar{\rho})(\gamma+\bar{\gamma})+(\mu-\bar{\mu})(\epsilon+\bar{\epsilon})=0. \tag{3.92}$$

It follows from combining this equation with Eq. (3.11a) that either

$$\bar{\mu}-\rho+\gamma+\bar{\gamma}-\epsilon-\bar{\epsilon}=0, \tag{3.93}$$

or, if $\bar{\mu}-\rho+\gamma+\bar{\gamma}-\epsilon-\bar{\epsilon}\neq 0$, then

$$\mu+\bar{\mu}+2\gamma+2\bar{\gamma}=0. \tag{3.94}$$

Case IIIA: $\bar{\mu}-\rho+\gamma+\bar{\gamma}-\epsilon-\bar{\epsilon}=0$.

Equation (3.93) implies

$$\bar{\rho}-\rho=\mu-\bar{\mu}, \tag{3.95}$$

and, consequently, Eq. (3.22) reduces to

$$(\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma})(\rho-\bar{\rho}+\bar{\mu}-\mu)=0. \tag{3.96}$$

The case when $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$ has already been considered, and, therefore, we shall assume $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}\neq 0$ so that $\rho-\bar{\rho}+\bar{\mu}-\mu=0$, which in conjunction with Eq. (3.94), yields

$$\rho=\bar{\rho},\quad \mu=\bar{\mu}. \tag{3.97}$$

Consideration of $[\delta,\Delta+D]w$ together with Eqs. (3.11), (3.97), and NP Eqs. (4.2) leads to

$$(1-3\dot{p})\bar{\nu}+(1+3\dot{p})\bar{\pi}=0. \tag{3.98}$$

Next, applying the δ operator to Eq. (3.93) eventually gives $\bar{\nu}=\bar{\pi}$ and, therefore, it follows from Eq. (3.98) that $\nu=\pi=0$, which is impossible since $\Psi_3\neq 0$.

Case IIIB: $\bar{\mu}-\rho+\gamma+\bar{\gamma}-\epsilon-\bar{\epsilon}\neq 0$.

In this case,

$$\rho+\bar{\rho}+2(\epsilon+\bar{\epsilon})=0. \tag{3.99}$$

Consideration of $[\delta,\Delta+D]w$ and $[\delta,D]w$ leads to

$$(\bar{\nu}+\bar{\pi})(\rho-\bar{\rho}+\mu-\bar{\mu})=0,$$

where use has been made of Eqs. (3.91), (3.92), (3.94), (3.99), and NP Eqs. (4.2). Now, if $\bar{\pi}+\bar{\nu}\neq 0$, then $\rho-\bar{\rho}+\mu-\bar{\mu}=0$ and it follows from Eq. (3.22) that we need only consider $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}\neq 0$ with $\rho=\bar{\rho}$, $\mu=\bar{\mu}$. However, these conditions immediately yield $\bar{\mu}-\rho+\gamma+\bar{\gamma}-\epsilon-\bar{\epsilon}=0$, which contradicts our original assumption, and thus this case is impossible. On the other hand, if $\bar{\nu}+\bar{\pi}=0$, then from $[\delta,\Delta+D]w$ we obtain the condition $\bar{\nu}(\rho+\mu)=0$, where we have used Eqs. (3.91), (3.94), (3.99), and a nonzero factor $w+p$ has been canceled throughout. The case when $\nu=0$ is impossible since $\Psi_3\neq 0$. Next, if $\rho+\mu=0$, then $\rho+\bar{\rho}+\mu+\bar{\mu}=0$, which implies $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$, which contradicts our original assumption. This completes the proof of the second part of the theorem; i.e., $u_{[a}l_bn_{c]}=0 \Rightarrow \theta=0$. A summary of the above results in the different subcases, is given in the Appendix.

IV. DISCUSSION

The results presented lend weight to the conjecture that general relativistic, shear-free perfect fluids which obey a barotropic equation of state are either nonexpanding or irrotational. It should be stressed that we have only shown the conjecture to hold in certain Petrov type III space-times which possess special alignment conditions. The general type III case is still proving to be elusive, due to the complexity of the resulting intermediate computations. Indeed, even with considerable increase in computer memory, the resulting "intermediate swell" of the integrability conditions is at certain stages too large for the algebraic computing system Maple to handle. However, there is some hope that it is possible to overcome this difficulty since the "swell" is, in general, dependent on the order with which preceding integrability conditions are obtained and used to simplify subsequent ones. On a separate issue, it appears from a search of the literature that there are no known type III, shear-free perfect fluid solutions of the Einstein field equations. In fact, we only know of one type III, perfect fluid solution, as given by Allnutt,[15] and the fluid has necessarily nonzero shear. Therefore, it is still not known whether shear-free solutions for type III space-times exist. In this regard the analysis presented here is also useful in that it does provide a number of possible avenues (Cases IA, IBib, IIB for when $\epsilon+\bar{\epsilon}+\gamma+\bar{\gamma}=0$ and IB, II, IIIA, IIIB for $\Psi_4=0$) leading to such shear-free solutions, if they exist with the additional alignment assumptions.

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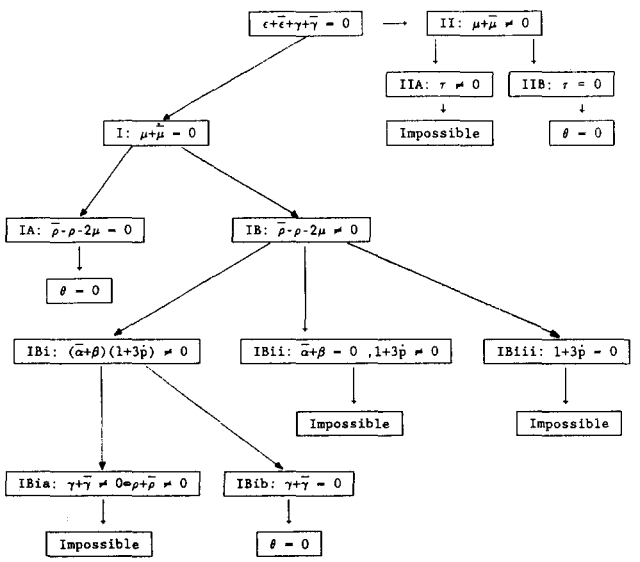
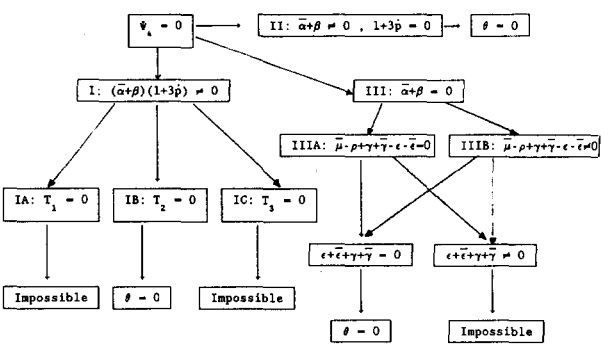
APPENDIX: SUMMARY OF RESULTS





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Reliability of perturbation theory in general relativity

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The relation between perturbation theory and exact solutions in general relativity is tackled by investigating the existence and properties of smooth one-parameter families of solutions. On the one hand, the coefficients of the Taylor expansion (in the parameter) of any given smooth family of solutions necessarily satisfy the hierarchy of perturbation equations. On the other hand, it is the converse question (does any solution of the perturbation equations come from Taylor expanding some family of exact solutions ?) which is of importance for the mathematical justification of the use of perturbation theory. This converse question is called the one of the "reliability" of perturbation theory. Using, and completing, recent results on the characteristic initial value problem, the local reliability of perturbation theory for general relativity in vacuum is proven very generally. This result is then generalized to the Einstein–Yang–Mills equations (and therefore, in particular, to the Einstein–Maxwell ones). These local results are then partially extended to global ones by: (i) proving the existence of semiglobal vacuum space-times (respectively, Einstein–Yang–Mills solutions) which are stationary before some retarded time u_0, and radiative after u_0, and which admit a smooth conformal structure at future null infinity; and (ii) constructing smooth one-parameter families of such solutions whose Taylor expansions are of the "multipolar post-Minkowskian" type which has been recently used in perturbation analyses of radiative space-times.

I. INTRODUCTION

A large body of knowledge is now available about existence and uniqueness theorems for Einstein field equations. There is also a vast literature, of varying degree of clarity and rigor, on approximation methods in general relativity. However, very little is known about the relation between the two approaches, which is unfortunate because the comparison between Einstein's theory and observations is almost completely based on approximation techniques. The mathematical result coming closest to building a bridge between existence theorems and one type of approximation method is Theorem 3 of Christodoulou and Schmidt.[1] However, this theorem concerns only the (harmonically) *reduced* Einstein equations, and assumes a *prescribed* matter source, as well as very special (trivial) Cauchy data for the gravitational field. Therefore, this theorem does not, per se, provide a mathematical justification for any actual approximation scheme in general relativity. By contrast, in the present paper, we shall provide a rigorous mathematical justification for a type of approximation scheme which is of use in practical applications.[2]

One can distinguish three main types of approximation schemes: post-Newtonian ones (where one solves at each step Poisson equations), post-Minkowskian ones (where one solves inhomogeneous d'Alembert equations), and the general class of perturbation expansions around a curved background. In all three types the nonlinearities of Einstein's field equations are recursively taken into account. In this paper we shall consider both the general perturbation theory, and its particular post-Minkowskian case (flat background), when applied to vacuum gravitational fields, i.e., to solutions of the homogeneous Einstein equations: $R_{ab}(g) = 0$ (Ref. 3). Because of the practical impossibility, in general, to solve in closed-form inhomogeneous wave equations on *curved* backgrounds the general perturbation theory is rarely used beyond its first, linearized, level. On the other hand, Blanchet and Damour[2] have recently shown explicitly how to construct to all nonlinearity orders a formal post-Minkowskian algorithm that aims at describing "the general field outside the source." The relation between such formal solutions and exact solutions of the field equations has been, up to now, left open. The purpose of this paper is to study this relation, and, surprisingly, we shall be able to give a simple (favorable) answer concerning the mathematical status of general perturbation expansions of the vacuum Einstein equations. We shall then generalize this result to the Einstein–Yang–Mills equations (which include the Einstein–Maxwell ones as a particular case). We shall also indicate how our method of proof can be applied to the Einstein–Euler equations.

The key notion is the one of a "curve of solutions" of the field equations, i.e., a one-parameter family of metrics $g(\lambda)$, where λ is a real parameter. It is now quite common to discuss linearized fields in relation to "the tangent to a C^1 curve of solutions."[4] This discussion has two aspects: First, the tangent, $h_{(1)} := [dg(\lambda)/d\lambda]_{\lambda=0}$, to a C^1 curve of solutions is clearly seen to be a linearized field, i.e., a solution of the

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linearized field equations expanded around the background $g_{(0)} := [g(\lambda)]_{\lambda=0}$, and, second, an important mathematical question is to know whether the converse is true. The latter question (is every solution of the linearized field equations the tangent to some curve of exact solutions ?) is often referred to as the one of "linearization stability."[4] In this paper we shall be concerned with the generalization of this setting to the C^∞ case.[5] The first aspect of the C^1 discussion above extends itself without difficulty to the result that the sequence of higher derivatives, say $h_{(n)} := (n!)^{-1} \times [d^n g(\lambda)/d\lambda^n]_{\lambda=0}$, of a smooth curve of solutions necessarily satisfies the usual hierarchy of equations associated with the fully expanded perturbation theory around the background $g_{(0)} := g(0)$ (see Sec. II below for details).

Therefore, the first insight is that a smooth curve of solutions determines a solution of the hierarchy of perturbation equations. This raises the first mathematical question of the existence of C^∞ one-parameter families of solutions of Einstein's equations (the usual discussions of the stability of Einstein equations, see, for example, Ref. 4 , consider explicitly only low orders of differentiability, C^0 or C^1). This question can be broken up into two subquestions: the existence of C^∞ one-parameter families of solutions of the constraint equations, and, the preservation of the smoothness in λ by the map going from the data to the solution (the so-called "Cauchy map"). The latter subquestion, that concerns the (hyperbolic) evolution part of Einstein's vacuum field equations, has (locally) a positive answer for data that are C^∞ jointly in λ and in the coordinates. This follows, for instance, from a general theorem of Choquet-Bruhat[6] about the C^p differentiability (in suitable Sobolev spaces) of the Cauchy map. Alternatively, this can be shown by using some of the results of Hamilton,[7] or, without using the heavy machinery of "tame Fréchet spaces," by an elegant trick due to Rendall.[8] The former subquestion (of showing the existence of smooth families of solutions of the constraint equations) is easier to tackle for the characteristic initial value problem rather than for the usual spacelike Cauchy problem. Indeed, Rendall[8] has proven recently an existence and uniqueness theorem for the characteristic initial value problem for Einstein vacuum equations, which includes the preservation of the smoothness in λ from the (characteristic) data to the solution. This way one can avoid (in local questions) the difficulties linked with the usual elliptic constraint equations, and construct smooth families as solutions of a characteristic problem. We shall generalize this approach to the Einstein–Yang–Mills equations (see Sec. III below).

Having learned that there exist many smooth one-parameter families (and therefore many corresponding solutions of the hierarchy of perturbation equations), we are naturally led, in analogy with the linearization stability problem, to ask whether any solution of the hierarchy of perturbation equations comes from some family of exact solutions. It is convenient at this point to introduce a specific terminology in order to avoid lengthy periphrases. We shall say that a hierarchy of perturbation equations (for some nonlinear problem) is *reliable*[9] if every solution of these equations, say $(h_{(1)}, h_{(2)}, \ldots, h_{(n)}, \ldots)$, comes from differentiating a smooth one-parameter family of exact solutions of the original nonlinear problem [i.e., $\exists g(\lambda); \forall n, h_{(n)} = (n!)^{-1}[d^n g(\lambda)/d\lambda^n]_{\lambda=0}$]. This terminology is well adapted to what constitutes the main motivation for posing such a mathematical problem, namely to ensure that the formal perturbation series used in comparing a theory with the observations is physically "reliable" for sufficiently small values of the expansion parameter because it is asymptotic when $\lambda \to 0$ to some exact solution:

$$\exists g(\lambda); \forall N, g_{(0)} + \lambda h_{(1)} + \cdots + \lambda^n h_{(n)} + \cdots + \lambda^N h_{(N)} = g(\lambda) + O(\lambda^{N+1}).$$

One of the main results of the present paper will be to prove that, locally, the perturbation theory for the vacuum Einstein equations is always reliable[10] (note that this does not imply global reliability). This is good news for, e.g., the multipolar post-Minkowskian expansion scheme of Ref. 2. It even leads to the possibility of expressing the difference between the Nth order formal expansion and the exact solution as the remainder term of a Taylor expansion. However, this remainder term depends on the values of the $(N+1)$th derivative at nonzero values of the parameter; in the present instance this means on some $(N+1)$th field on a *curved* metric. This is rarely under control. The strongest explicit statement that one can make is that, on some fixed compact space-time region, say K, there will always exist, for any finite integer N, two (unfortunately unknown) numbers λ_0 and C, such that

$$\lambda < \lambda_0 \Rightarrow \sup_{x \in K} |g_{(0)} + \lambda h_{(1)} + \cdots + \lambda^N h_{(N)} - g(\lambda)| < C\lambda^{N+1}.$$

So far we talked mainly about Einstein's vacuum equations. The fact that differentiable families of exact solutions provide solutions to perturbation equations extends trivially to more general cases. The difficulty is to prove, on the one hand, the existence of smooth families of exact solutions, and, on the other hand, the fact that every solution of the hierarchy of perturbation equations comes from differentiating a smooth curve of exact solutions. As will be clear from the method of proof that we shall use in Sec. IV, the result of reliability of perturbation theory extends to all the cases where a characteristic initial value treatment in the manner of Ref. 8 works (see end of Sec. IV). This includes, as we shall show, the Einstein–Maxwell and the Einstein–Yang–Mills cases. Einstein's equations coupled to a barotropic perfect fluid can also be treated locally in any connected region where $\rho + p \neq 0$. For finite bodies (having spatially compact supports) one is, however, confronted with the difficulty that no existence theorem is known.

It might be worth pointing out that a description of post-Newtonian-type expansions similar to that given here of post-Minkowskian ones is not presently possible. The basic reason is that if one treats the Newtonian limit as a limit of families of solutions of Einstein's equations, the limit is singular from the point of view of the differential equation (see, e.g., Ref. 11). Therefore, besides explicit examples, nothing is known in general about the reliability of post-Newtonian expansions.

Finally, we shall show also that, although our reliability

results are purely local (i.e., valid in a compact domain of $\mathscr{R}^4$), they can be used to relate post-Minkowskian expansions and exact solutions on physically infinite domains. This will be done by proving that certain radiative semiglobal vacuum solutions (whose existence was assumed as a motivation in Ref. 2) actually do exist and admit a piece of conformally regular future null infinity with spherical sections. In particular, we can construct smooth families of such solutions whose Taylor expansions are exactly of the multipolar-post-Minkowskian type studied in Ref. 2. Our construction generalizes also to the Einstein–Yang–Mills case. This is a nice example of how a combination of various general theorems [local characteristic initial value problem, Friedrich's regularization[12] (see, also, Ref. 13) of the conformal Einstein equations, general stability of symmetric hyperbolic systems] can provide the existence of a class of exact solutions with physically interesting properties.

The paper is organized as follows: Sec. II explicates in detail the relation between the Taylor series of a smooth curve of solutions and the hierarchy of perturbation equations. In Sec. III we show (after Rendall's work[8]) how to construct (locally) smooth families of solutions via the characteristic initial value problem. We treat both the vacuum equations and the Einstein–Yang–Mills ones. We mention also briefly how to proceed via the usual Cauchy problem. In Sec. IV we establish our main results: the local reliability of the perturbation theory for Einstein's vacuum equations, as well as for Einstein–Yang–Mills ones. In Sec. V we prove the existence of smooth families of certain radiative semiglobal solutions in a way that allows us to extend our reliability results of post-Minkowskian expansions to a physically infinite domain.

II. TAYLOR EXPANSIONS OF SMOOTH ONE-PARAMETER FAMILIES OF SOLUTIONS

Let us consider a smooth one-parameter family (or curve) of metrics: $g(\lambda)$. As we shall use below local existence theorems in C^∞ settings, it will be enough for our purpose to define such a C^∞ curve of metrics simply by assuming that the metric components in some chart, $g_{ab}(x^c,\lambda)$, are jointly C^∞ in the coordinates and in the parameter on some open domain $U\times I\subset\mathscr{R}^5$ (where the open interval $I\subset\mathscr{R}$ contains zero). A coordinate-independent description of such families has been given by Geroch.[14] As we are dealing with purely local matters in this section we can avoid this formalization; it is, however, useful to have in mind the corresponding picture of a five-dimensional manifold, coordinatized by (x^c,λ).

The smoothness in λ allows one to make finite Taylor expansions of any order N in powers of λ:

$$g_{ab}(\lambda)=g_{(0)ab}+\lambda h_{(1)ab}+\lambda^2 h_{(2)ab}+\cdots+\lambda^N h_{(N)ab}+\lambda^{N+1}k_{(N)ab}(\lambda). \tag{1}$$

The zeroth term, $g_{(0)ab}(x^c)=[g_{ab}(x^c,\lambda)]_{\lambda=0}$, and the expansion coefficients $h_{(n)ab}$ are C^∞ functions of the coordinates x^c. The latter are given by the derivatives

$$h_{(n)ab}(x^c)=\frac{1}{n!}\left[\frac{\partial^n g_{ab}(x^c,\lambda)}{\partial\lambda^n}\right]_{\lambda=0}. \tag{2}$$

The remainder term is the product of λ^{N+1} by a C^∞ function of x^c and λ:

$$k_{(N)ab}(x^c,\lambda)=\frac{1}{N!}\int_0^1 d\alpha(1-\alpha)^N\left[\frac{\partial^{N+1}g_{ab}}{\partial\lambda^{N+1}}\right](x^c,\alpha\lambda). \tag{3}$$

The Ricci tensor R_{ab} is pointwise a smooth (in fact analytic) function of the metric components and their derivatives up to order 2. Inserting, therefore, the truncated expansion (1) into the definition of the Ricci tensor one obtains the Taylor expansion of $R_{ab}(\lambda)$: $=R_{ab}[g(\lambda),\partial g(\lambda),H\partial^2 g(\lambda)]$,

$$R_{ab}(\lambda)=R_{(0)ab}+\lambda R_{(1)ab}+\lambda^2 R_{(2)ab}+\cdots+\lambda^N R_{(N)ab}+\lambda^{N+1}S_{(N)ab}(\lambda), \tag{4}$$

where the zeroth term is the Ricci tensor of $g_{(0)ab}$,

$$R_{(0)ab}=R_{ab}[g_{(0)}], \tag{5}$$

while the expansion coefficients are successively: The linearized Ricci tensor around the metric $g_{(0)}$,

$$R_{(1)ab}=L[g_{(0)}]h_{(1)ab}, \tag{6a}$$

and, for $n\geqslant 2$, nonlinear expressions of the type:

$$R_{(n)ab}=L[g_{(0)}]h_{(n)ab}-N_{(n)ab}[g_{(0)},h_{(1)},\ldots,h_{(n-1)}]. \tag{6b}$$

In Eq. (6b) L denotes the same linear second-order differential operator as in Eq. (6a) (linearized Ricci operator around $g_{(0)}$), while the $N_{(n)}$'s are nonlinear polynomials of the $h_{(i)}$'s and of their derivatives up to order 2.

Let us now assume that all members of the family $g_{ab}(\lambda)$ satisfy Einstein's vacuum field equations: $R_{ab}[g(\lambda)]=0$. This implies, by differentiating with respect to λ, that all the coefficients $R_{(n)ab}$, $n\geqslant 0$, must vanish. Hence, the metric $g_{(0)}$ is Ricci-flat,

$$R_{ab}[g_{(0)}]=0, \tag{7}$$

and the $h_{(n)}$'s automatically satisfy a hierarchy of linear equations:

$$L[g_{(0)}]h_{(1)ab}=0, \tag{8a}$$

$$n\geqslant 2\Rightarrow L[g_{(0)}]h_{(n)ab}=N_{(n)ab}[g_{(0)},h_{(1)},\ldots,h_{(n-1)}]. \tag{8b}$$

Because of the uniqueness of the Taylor expansion, the hierarchy (7) and (8) is exactly the same as the usual equations of perturbation theory, obtained by inserting a formal power series, $g_{ab}=g_{(0)ab}+\lambda h_{(1)ab}+\cdots+\lambda^n h_{(n)ab}+\cdots$, into Einstein's vacuum field equations. We shall discuss later one way of describing the general solution of this perturbation hierarchy. At this point let us only say that the only case which is amenable to an explicit treatment is the post-Minkowskian case, i.e., $g_{(0)ab}=f_{ab}$, the flat Minkowski metric. Moreover, if one uses harmonic coordinates the hierarchy consists (besides a sequence of "harmonicity constraints") of a sequence of inhomogeneous d'Alembert equations whose "source terms" are calculable from the previous itera-

tions. Such a hierarchy is the basis of many approximation schemes in general relativity.

It is clear that the one-way link, family of exact solutions→solution of perturbation hierarchy, extends to very general nonlinear problems (it is sufficient that the field equations be smooth functions of the field variables, and their derivatives up to some finite order). This includes, for instance, the Einstein–Yang–Mills equations, that we shall consider below.

III. ON THE EXISTENCE OF SMOOTH ONE-PARAMETER FAMILIES OF SOLUTIONS

Many of the known exact vacuum solutions of Einstein's equations depend smoothly on at least one parameter. The Schwarzschild and Kerr solutions are well-known examples. The purpose of this section is to demonstrate that this is a rather general property. To keep the notation simple we shall consider only one-parameter families; however, everything we say is easily extended to the multiparameter case.

Solutions of the field equations are determined by data. Hence, the obvious questions are: Do smooth curves of data exist?, and, do smooth curves of data determine smooth curves of solutions? One can ask these questions for the usual spacelike Cauchy problem (with elliptic constraints on the data), as well as for the characteristic initial value problem (where some analogs of the constraints reduce to ordinary differential equations). We give a complete treatment of the characteristic case and make some remarks about the Cauchy case. We shall first consider Einstein's vacuum equations, and then generalize the results to the Einstein–Yang–Mills equations.

For Einstein's vacuum equations, Rendall[8] has recently presented a new treatment of the local characteristic initial value problem (in a C^∞ setting) that contains the answers to our questions. (In the next section we shall complete his treatment by giving the explicit expressions of the hierarchical system of ordinary differential equations that play the role of the constraints). Let us describe first the coordinate system in which the existence and uniqueness theorem is proved.

Definition 1 ("Standard coordinates"[8]): Let us be given a (smooth) Lorentz metric (signature $-+++$) and a connected (smooth) spacelike two-surface S. Let N_1 and N_2 be the two null hypersurfaces generated by the null geodesics issued orthogonally from S (so that $S = N_1 \cap N_2$). A coordinate system x^a is called standard with respect to (g,S) if: (i) the equation of N_1 is $x^2 = 0$, and the null generators of N_1 are the curves $x^2 = \text{const}$, $x^A = \text{const}$ $(A = 3,4)$, with x^1 being an affine parameter along them; (ii) same requirement when exchanging the indices 1 and 2; (iii) on S (i.e., when $x^1 = x^2 = 0$) $g_{12} = -1$; (iv) the coordinates x^a are harmonic in the future and the past of S.[15]

To construct (locally) such coordinates starting from (g,S) one can first Lie-drag along N_1 a coordinate system x^A $(A = 3,4)$ defined on S by means of an affinely normalized null vector field l normal (and tangent) to N_1. Then one Lie-drags x^A along N_2 by means of a correspondingly defined null vector field n on N_2 (with the normalization $l \cdot n = -1$ on S). One then sets $x^2 = 0$ and $l = \partial/\partial x^1$ on N_1, and, $x^1 = 0$ and $n = \partial/\partial x^2$ on N_2. This defines the values taken by the four coordinates $(x^a) = (x^1, x^2, x^A)$ on $N_1 \cup N_2$. These values can be taken as (smooth) characteristic initial data for the wave equation $\Box_g x^a = 0$ (harmonicity condition) and thereby be propagated to the future and the past of S.

In general, the existence of such standard coordinates will be guaranteed only in a neighborhood of S (e.g., because of possible caustics in N_1 or N_2). Moreover, if S cannot be covered by a single coordinate patch (x^A) one will need to use several overlapping standard coordinate systems to study the characteristic problem based on S, N_1, N_2.

Theorem 3 in Ref. 8 establishes the following.

Theorem 1 (Rendall[8]): Existence and uniqueness of local C^∞ solutions in standard coordinates of the characteristic initial value problem for Einstein's vacuum field equations.

Notation: Let in $\mathscr{R}^4 = \{(x^a),\ a = 1,2,3,4\}$ the hyperplane $x^1 = 0$ be denoted by N_2, the hyperplane $x^2 = 0$ by N_1, and the two-plane $x^1 = x^2 = 0$ by $S (S = N_1 \cap N_2)$. Let G denote the region $x^1 x^2 \geqslant 0$.

A function on $N_1 \cup N_2$ will be called smooth if its restrictions to N_1 and N_2 are smooth, and if it is continuous (at $S = N_1 \cap N_2$). A function on G will be called smooth if it can be extended to a smooth function on $\mathscr{R}^4$.

Data: Let $\tilde{\gamma}_{AB}$ $(A,B = 3,4)$ be smooth functions on $N_1 \cup N_2$ which make up a symmetric positive definite matrix with determinant nowhere vanishing.

Let five C^∞ functions, denoted $\overline{\omega}$, $\overline{\omega_1}$, $\overline{\omega_2}$, $\overline{\beta_{A1}}$ $(A = 3,4)$, be given on S.

Statements: Given the data there exists an open neighborhood U of S, a unique smooth function ω on $(N_1 \cup N_2) \cap U$ and a unique smooth Lorentz metric g_{ab} on $G \cap U$ such that: (i) g_{ab} satisfies the vacuum Einstein equations on $G \cap U$; (ii) the given coordinates x^a on $\mathscr{R}^4$ are standard coordinates for g_{ab}; (iii) $g_{AB} = \omega \tilde{\gamma}_{AB}$ on $N_1 \cup N_2$; and (iv) $\omega = \overline{\omega}$, $\omega_{,1} = \overline{\omega_1}$, $\omega_{,2} = \overline{\omega_2}$, and $g_{2A,1} = \overline{\beta_{A1}}$ on S.

Moreover, if the data depend smoothly on one (or several) parameters, then so does the solution.

We see that this theorem guarantees the existence of local smooth one-parameter (or several-parameter) families of vacuum solutions in abundance. In the formulation of the theorem in Ref. 8 it was assumed that $\det(\tilde{\gamma}_{AB}) = 1$. This is, however, irrelevant, and we shall see later that it can be useful in applications not to have to normalize the determinant of $\tilde{\gamma}_{AB}$ to unity. Let us note also that the data given on N_1 and N_2 are given on both halves of N_1 and N_2 (with respect to S), so that the solution is determined both in the future $(x^1 \geqslant 0$ and $x^2 \geqslant 0)$ and the past $(x^1 \leqslant 0$ and $x^2 \leqslant 0)$ of S. If one is interested only in determining g_{ab} in the future of S, it is sufficient to give data on the "upper halves" of N_1 and N_2. However, one must still enforce that the data are "smooth" on these (closed) half-hyperplanes which means extendable to C^∞ functions on the full hyperplanes.

Before generalizing the characteristic approach to the coupled Einstein–Yang–Mills system, let us discuss briefly

how one can prove the existence of smooth families of vacuum solutions via the usual spacelike Cauchy problem. The subquestion of whether smooth families of Cauchy data evolve into smooth families of solutions has (locally) a positive answer for data that are C^∞ jointly in λ and in the coordinates. As remarked in the Introduction, this follows from Theorem 3 of Ref. 6 about the finite differentiability (in suitable Sobolev spaces) of the Cauchy map. This can be shown also by using the setting of "tame Fréchet spaces,"[7] or, more simply, by using Rendall's trick[8] of considering λ as a new coordinate in a symmetric hyperbolic system. It remains then to prove the existence of smooth families of solutions of the (elliptic) constraints. Let us only show how this can be done in particular cases.

If we consider time-symmetric Cauchy data, the second fundamental form of the Cauchy hypersurface vanishes and only the "energy constraint" has to be considered. The latter can be reduced to the Lichnerowicz equation:

$$\Delta_h \Phi - \tfrac{1}{8}\Phi R\,[h\,] = 0. \tag{9}$$

A positive definite three-metric $h_{\alpha\beta}$ ($\alpha,\beta = 1,2,3$) can be chosen freely and if Φ satisfies the linear equation (9) the three-metric $\Phi^4 h_{\alpha\beta}$, together with a zero second fundamental form, is a solution of the constraints.[16] To construct local solutions we can choose smooth families of three-metrics $h_{\alpha\beta}$ and pose a local Dirichlet problem. The smoothness of the solution, including in λ, is guaranteed by the treatment of linear elliptic equations in the setting of tame Fréchet spaces by Hamilton.[7] In the not time-symmetric case, the existence of local smooth families of solutions of the constraints follows from a theorem by Rendall.[17] He shows that smooth families of solutions of the linearized constraints are tangent to smooth families of solutions of the nonlinear constraints.

Let us now deal with the coupled Einstein–Yang–Mills system. We then consider a Lie group G and a principal G bundle P over a four-dimensional manifold M. As we shall mainly be interested in local questions, we will assume that the bundle is trivial. A connection on P can then be described as a covectorial field on M, $\mathbf{A}_a$, taking its values in the Lie algebra $\mathcal{G}$ of G (we shall use boldface letters to denote elements of $\mathcal{G}$). The fields of the Einstein–Yang–Mills system are then a (smooth, real-valued) Lorentz metric g_{ab} and a (smooth, Lie-algebra valued) "gauge potential," $\mathbf{A}_a$. Let us first define a convenient "gauge" in which an existence and uniqueness theorem can be proved.

Definition 2 "Standard gauge": Given a two-surface S (and its associated null hypersurfaces N_1 and N_2, like in Definition 1 above) a gauge (i.e., a combined choice of a trivialization of P and of a coordinatization of M) is called standard with respect to S if:

(a) the base coordinates x^a are "standard" with respect to S in the sense of Definition 1. In particular, this means that the "harmonicity conditions" $\Gamma_a = 0$ are satisfied, where Γ_a is defined as

$$\Gamma_a := g^{bc}(g_{ab,c} - \tfrac{1}{2}g_{bc,a});$$

(b) $\mathbf{A}_1 \equiv \mathbf{A}_a l^a = 0$ on N_1 (generated by the null vector field l), and, correspondingly, $\mathbf{A}_2 = 0$ on N_2;

(c) the "Lorentz condition" $\Delta = 0$ is satisfied, where Δ is defined as

$$\Delta := g^{ab}\,\partial_a\,\mathbf{A}_b$$

($\Delta = 0$ is equivalent, in harmonic coordinates, to $\nabla^a \mathbf{A}_a = 0$ where ∇ denotes the Levi-Civita connection).

It is easy to check that such a gauge can always be (locally) constructed. Indeed, having constructed standard coordinates x^a (see Definition 1), the algebraic conditions (b) lead to ordinary differential equations within N_1 and N_2 for the gauge transition mapping, say φ (going from any given gauge to the looked for standard gauge). This defines values for the transition mapping φ on $N_1 \cup N_2$. These values can then be taken as characteristic initial data for the hyperbolic evolution equation (with principal part $g^{ab}\,\partial_{ab}\,\varphi$) that is entailed by the Lorentz condition. This propagates φ to the future and the past of S.

We shall now establish the following theorem.

Theorem 2: Existence and uniqueness of local C^∞ solutions in standard gauge of the characteristic initial value problem for the Einstein–Yang–Mills system.

Notation: Notation of Theorem 1, and in addition let

$$\mathbf{F}_{ab} := \partial_a \mathbf{A}_b - \partial_b \mathbf{A}_a + [\mathbf{A}_a, \mathbf{A}_b],$$

$$\mathbf{Y}^a := \nabla_b \mathbf{F}^{ab} + [\mathbf{A}_b, \mathbf{F}^{ab}],$$

$$\tau_{ab} := \mathbf{F}_{as} \cdot \mathbf{F}_b{}^s - \tfrac{1}{4}\, g_{ab}\, \mathbf{F}_{rs} \cdot \mathbf{F}^{rs},$$

where the square brackets denote the Lie-algebra product, and the dot the Cartan–Killing scalar product.

Data: Metric data as in Theorem 1 (i.e., $\tilde{\gamma}_{AB}$ on $N_1 \cup N_2$, and $\bar{\omega}$, $\overline{\omega_1}$, $\overline{\omega_2}$, $\overline{\beta_{A1}}$ on S). For gauge potential data, let $\tilde{\mathbf{A}}_B$ ($B = 3,4$) be smooth (Lie-algebra-valued) functions on $N_1 \cup N_2$, and let $\bar{\sigma}$ be a smooth (Lie-algebra-valued) function on S.

Statements: Given the data there exists an open neighborhood U of S, a unique smooth function ω on $(N_1 \cup N_2) \cap U$, a unique smooth Lorentz metric g_{ab} on $G \cap U$ and a unique smooth gauge potential $\mathbf{A}_a$ on $G \cap U$ such that: (i) $(g_{ab}, \mathbf{A}_a)$ satisfies the Einstein–Yang–Mills equations on $G \cap U$:

$$R_{ab} - k\tau_{ab} = 0,$$

$$\mathbf{Y}_a = 0,$$

in which k denotes the combined gravitational-gauge-field coupling constant (proportional to G/g^2); (ii) the solution $(g_{ab}, \mathbf{A}_a)$ is expressed in a standard gauge; (iii) on $N_1 \cup N_2$: $g_{AB} = \omega \tilde{\gamma}_{AB}$ and $\mathbf{A}_B = \tilde{\mathbf{A}}_B$; and (iv) on S: $\omega = \bar{\omega}$, $\omega_{,1} = \overline{\omega_1}$, $\omega_{,2} = \overline{\omega_2}$, $g_{2A,1} = \overline{\beta_{A1}}$, and $\mathbf{F}^1{}_1 = \bar{\sigma}$.

Moreover, if the data depend smoothly on one (or several) parameters, then so does the solution.

Proof: Given the data, one defines values for all the components of the metric and gauge potential (in a standard gauge) on $N_1 \cup N_2$ by integrating the ordinary differential equations ("characteristic constraints") explicitly written down in the next section [Eqs. (28), taken with $\mathbf{A}_B = \tilde{\mathbf{A}}_B$, and the corresponding equations on N_2]. The initial values (on S) for these ordinary differential equations (written both on N_1 and N_2) are successively: $\omega = \bar{\omega}$, $\omega_{,1} = \overline{\omega_1}$,

$\omega_{,2} = \overline{\omega_2}$; $g_{12} = -1$; $\mathbf{F}^1{}_1 = \bar{\sigma}$, $\mathbf{F}^2{}_2 = -\bar{\sigma}$ (on N_2); $g_{2A} = 0$, $g_{2A,1} = \overline{\beta_{A1}}$, $g_{1A} = 0$, $g_{1A,2} = -\overline{\beta_{A1}} + [\gamma_A]_S$; $g_{22} = 0$, $g_{22,1} = -[\theta_{N_2}]_S$, $g_{11} = 0$, $g_{11,2} = -[\theta_{N_1}]_S$; $\mathbf{A}_2 = 0$, $\mathbf{A}_1 = 0$.

These values, $[g_{ab}]_{N_1 \cup N_2}$, $[\mathbf{A}_a]_{N_1 \cup N_2}$, are then taken as initial data for the characteristic initial value problem of the following gauge-reduced Einstein–Yang–Mills system:

$$R^H_{ab} - k\tau_{ab} = 0,$$

$$\mathbf{Y}^L_a = 0,$$

in which one has defined

$$R^H_{ab} := R_{ab} - \tfrac{1}{2}(\partial_a \Gamma_b + \partial_b \Gamma_a),$$

$$\mathbf{Y}^L_a := \mathbf{Y}_a - \partial_a \Delta.$$

This gauge-reduced system is a diagonal hyperbolic quasilinear evolution system for $(g_{ab}, \mathbf{A}_a)$ with principal part $(-\tfrac{1}{2}g^{rs}\partial_{rs}g_{ab}, -g^{rs}\partial_{rs}\mathbf{A}_a)$. By Theorem 1 of Ref. 8, there exists an open neighborhood U of S, and unique smooth functions $(g_{ab}, \mathbf{A}_a)$ on $U \cap G$ that solve this gauge-reduced system and coincide with the characteristic-constraints-defined initial values on $N_1 \cup N_2$. To prove that these functions $(g_{ab}, \mathbf{A}_a)$ satisfy also the gauge conditions on $U \cap G$ one then proceeds in three steps. First, one checks that the initial values on S, taken for the ordinary differential equations, ensure the vanishing of the gauge conditions Γ_a and Δ on S. Second, combining the constraints with the gauge-reduced field equations one gets linear homogeneous equations on $N_1 \cup N_2$ for Δ and Γ_a. More precisely, denoting $\partial_1 + \frac{1}{2}\theta$ by $\tilde{D}$, one gets successively on N_1: from the Yang–Mills equations $\tilde{D}\,\Delta = 0$ (and $\Delta = \mathbf{F}^1{}_1 - \sigma$), which, as $[\Delta]_S$ is known to vanish, ensures the vanishing of Δ (and $\mathbf{F}^1{}_1 - \sigma$) all over N_1; then, from the ω and α constraints, and $R^H_{11} - k\tau_{11} = 0$, $\tilde{D}\Gamma_1 = 0$ and $g = -\frac{1}{2}\Gamma_1$, which imply that $\Gamma_1 = g = 0$ on N_1 (where g is defined by $l^b \nabla_b l^a = g l^a$); then one gets similarly $\tilde{D}\Gamma_A = 0 \Rightarrow \Gamma_A = 0$ on N_1; and, finally, $\tilde{D}\Gamma_2 = 0 \Rightarrow \Gamma_2 = 0$ on N_1. Correspondingly, one gets also the vanishing of Δ and Γ_a on N_2. The final step consists of combining the gauge-reduced equations with the Bianchi identities (for both the gravitational and the gauge-field equations). This yields a linear homogeneous system for (Γ_a, Δ) with principal part $(g^{rs}\partial_{rs}\Gamma_a, g^{rs}\partial_{rs}\Delta)$. The uniqueness of the solution of the characteristic initial value problem for this system, guarantees the vanishing of Γ_a and Δ everywhere in $U \cap G$. Finally, the statement concerning smooth dependence on parameters follows, as in Theorem 1 above, from the trick[8] of adding the parameters as new coordinates in a symmetric hyperbolic system.

IV. LOCAL RELIABILITY OF PERTURBATION THEORY FOR EINSTEIN'S VACUUM FIELD EQUATIONS, AND FOR EINSTEIN–YANG–MILLS EQUATIONS

We have seen that a large class of smooth one-parameter families of solutions of Einstein's vacuum field equations exist locally, and that their successive Taylor coefficients satisfy the hierarchy of perturbation equations (7) and (8). It is natural to ask whether the converse is true. More precisely, the property for any solution of the hierarchy truncated at order N (resp. of the whole hierarchy) to coincide with the first N derivatives (resp. all derivatives) of a C^N (resp. C^∞) one-parameter family of solutions will be termed the "reliability up to the Nth order" (resp. "reliability to all orders") of the perturbation theory. This terminology is chosen in order to emphasize the importance of this question in the context of the use of a (partial) solution of the perturbation hierarchy as an "approximate solution of the equations."

If we take just the first Eq. (8a), and consider its local solutions, this question of "local reliability at first order" is often termed "local linearization stability." It was positively answered in Ref. 18. We shall first show in this section that the perturbation theory around any curved background for general relativity in vacuum is locally reliable to all orders. We shall then generalize this result to the Einstein–Yang–Mills system. More precisely, let us first prove the following theorem.

Theorem 3: Local reliability (to all orders) of the perturbation hierarchy for Einstein's vacuum field equations.

Let $h'_{(n)ab}(x'^c)$, with $1 \leqslant n \leqslant N$, be a (local) smooth solution of Eqs. (8) with $g'_{(0)ab}(x'^c)$ being some smooth Ricci-flat Lorentz metric. Then there exists (locally) a (nonunique) C^∞ one-parameter family of Ricci-flat metrics, $g'(\lambda)$, such that, in some coordinate system x'^c,

$$g'_{(0)ab}(x'^c) = [g'_{ab}(x'^c, \lambda)]_{\lambda = 0}$$

and

$$h'_{(n)ab}(x'^c) = \frac{1}{n!}\left[\frac{\partial^n g'_{ab}(x'^c, \lambda)}{\partial \lambda^n}\right]_{\lambda = 0}, \quad \text{for } 1 \leqslant n \leqslant N.$$

[Therefore, Eqs. (1) and (3) hold also.]

If one starts with a solution $h'_{(n)}$ for all orders, the same conclusion holds with a C^∞ family $g'(\lambda)$ which is still nonunique in general. [Then Eqs. (1) and (3) hold for any finite order N, but have, in general, no infinite order limit.]

Proof: Let us define a family of bicovariant tensors by the following finite sum:

$$^N g'_{ab}(x'^c, \lambda) := g'_{(0)ab}(x'^c) + \lambda h'_{(1)ab}(x'^c) + \lambda^2 h'_{(2)ab}(x'^c) + \cdots + \lambda^N h'_{(N)ab}(x'^c). \tag{10}$$

For λ small enough $^N g'(\lambda)$ will still be a Lorentz metric, so that Eq. (10) defines a smooth family of Lorentz metrics (henceforth, "smooth" or C^∞, will mean "locally C^∞ jointly in λ and in the coordinates"). As we saw in Sec. II, the hypothesis of the theorem implies that the Ricci tensor of this family, $^N R'_{ab}(\lambda) := R_{ab}[^N g'(\lambda)]$, satisfies

$$^N R'_{ab}(x'^c, \lambda) = \lambda^{N+1} S'_{(N)ab}(x'^c, \lambda), \tag{11}$$

for some smooth tensor $S'_{(N)ab}$.

Choose now a smooth family of (connected) two-surfaces S_λ, spacelike with respect to $^N g'(\lambda)$. As recalled in Sec. III, we can then construct standard coordinates with respect to $(^N g'(\lambda), S_\lambda)$, say $x^a = f^a(x'^b, \lambda)$. In these coordinates the equations of the two-surfaces S_λ are independent of λ and are simply that of the two-plane S of Theorem 1, namely, $x^1 = x^2 = 0$. The transformation functions $f^a(x'^b, \lambda)$ are (locally) constructed, first by integrating ordinary differential equations with smooth coefficients, and then by solving

wave equations with smooth coefficients, and smooth characteristic initial data given on coordinate-fixed null hypersurfaces ($x^1 = 0$ and $x^2 = 0$). Therefore, the results of Ref. 8 apply and guarantee that the $f^a(x'^b,\lambda)$ are smooth functions of x'^b and λ. Performing the (λ dependent) coordinate transformation $x^a = f^a(x'^b,\lambda)$, we obtain another representation of the family (10), say ${}^N g_{ab}(x^c,\lambda)$. The finite Taylor expansion of this smooth family leads to

$$
\begin{aligned}
{}^N g_{ab}(x^c,\lambda) = :& g_{(0)ab}(x^c) + \lambda h_{(1)ab}(x^c) \\
&+ \lambda^2 h_{(2)ab}(x^c) + \cdots + \lambda^N h_{(N)ab}(x^c) \\
&+ \lambda^{N+1} k_{(N)ab}(x^c,\lambda).
\end{aligned} \tag{12}
$$

The new expansion coefficients $g_{(0)ab}$, $h_{(n)ab}$, $1 \leqslant n \leqslant N$, still satisfy the perturbation hierarchy (7) and (8) because the Ricci tensor of ${}^N g_{ab}$ satisfies

$$
{}^N R_{ab}(x^c,\lambda) = \lambda^{N+1} S_{(N)ab}(x^c,\lambda), \tag{13}
$$

where the smooth tensor $S_{(N)ab}$ is just the coordinate transform of the $S'_{(N)ab}$ of Eq. (11).

Using Theorem 1 of Sec. III, let us now define (locally around S) a one-parameter family of solutions of Einstein's vacuum equations, say ${}^X g_{ab}(x^c,\lambda)$ (the upper prefix X standing for "exact"), as being, for each λ, the unique Ricci-flat metric in standard coordinates having as characteristic initial value data:

$$
\text{on } N_1 \cup N_2 : \tilde{\gamma}_{AB} := \left[{}^N g_{AB} \right]_{N_1 \cup N_2} \quad (A,B = 3,4), \tag{14a}
$$

$$
\text{on } S: \bar{\omega} := 1, \bar{\omega}_1 := 0, \bar{\omega}_2 := 0, \overline{\beta_{A1}} := \left[{}^N g_{2A,1} \right]_S. \tag{14b}
$$

From the last statement in Theorem 1, and the fact that the data depend [as ${}^N g(\lambda)$] smoothly on λ, we know that the Ricci-flat family ${}^X g(\lambda)$ will be smooth. We are going to prove that the successive derivatives, from the zeroth up to the Nth order, of ${}^X g(\lambda)$ coincide (over the local four-dimensional domain of definition of ${}^X g$) with the expansion coefficients of Eq. (12). Let us first remark that, by construction, the ${}^Z g(\lambda)$'s (where $Z = N$ or X) are expressed in standard coordinates for all λ's (in some open interval around zero). In particular, this is true for the zeroth expansion coefficient, ${}^Z g_{(0)} := {}^Z g(\lambda = 0)$. On the other hand, by definition [take $\lambda = 0$ in Eqs. (14)] the characteristic data that define ${}^X g_{(0)}$ are the ones induced by ${}^N g_{(0)}$ on $N_1 \cup N_2$ (with $\omega = 1$ all over $N_1 \cup N_2$). Because of the uniqueness part of Theorem 1, one has immediately the result that ${}^X g_{(0)} = {}^N g_{(0)}$ all over some four-dimensional local neighborhood $U \cap G$ of S (we shall henceforth denote simply by $g_{(0)}$ this common "background metric").

As for the higher derivatives, say ${}^Z h_{(n)}$ (where $Z = N$ or X), we know that they satisfy the perturbation equations (8). Moreover, they also satisfy (among others) four particular "gauge conditions" obtained by differentiating the λ-dependent harmonicity condition,

$$
{}^Z \Gamma_a(\lambda) := {}^Z g^{bc}(\lambda) \left[{}^Z g_{ab,c}(\lambda) - \tfrac{1}{2} {}^Z g_{bc,a}(\lambda) \right] = 0, \tag{15}
$$

which follows from the construction of both ${}^N g(\lambda)$ and ${}^X g(\lambda)$ in standard coordinates. These gauge conditions can be written in the form,

$$
\nabla_{(0)b} \left({}^Z h^b_{(n)a} - \tfrac{1}{2} {}^Z h^c_{(n)c} \delta^b_a \right) = F_{(n)a} \left[{}^Z h_{(1)}, \ldots, {}^Z h_{(n-1)} \right], \tag{16}
$$

where ${}^Z h^b_{(n)a} := g^{bc}_{(0)} {}^Z h_{(n)ac}$, where $\nabla_{(0)}$ is the Levi-Civita connection of $g_{(0)}$, and where $F_{(1)} = 0$. It is a well-known result in perturbation theory (see e.g., Ref. 4) that the use of the gauge conditions (16) in Eqs. (8) satisfied by the ${}^Z h_{(n)}$'s leads to show that the ${}^Z h_{(n)}$'s satisfy a hierarchy of linear inhomogeneous "wave equations" (with "wave operator" $\Box_{(0)L}$ the De Rham–Lichnerowicz Laplacian computed in the background metric $g_{(0)}$). If we consider the first step of the hierarchy, it satisfies the homogeneous wave equation

$$
\Box_{(0)L} {}^Z h_{(1)} = 0. \tag{17}
$$

Standard results for linear wave equations (see, e.g., Ref. 19) show that a solution of Eq. (17) is uniquely determined by giving oneself the values of the ${}^Z h_{(1)ab}$'s (for $a,b = 1,\ldots,4$) on $N_1 \cup N_2$ (which, by construction, are characteristic hypersurfaces for $g_{(0)}$). Therefore, if we can prove that ${}^N h_{(1)ab}$ is equal to ${}^X h_{(1)ab}$ (for $a,b = 1,\ldots,4$) on $N_1 \cup N_2$, this equality will be propagated also to the future and the past of $N_1 \cap N_2$. This will then imply that the difference ${}^N h_{(2)ab} - {}^X h_{(2)ab}$ satisfies again the homogeneous wave equation (17). By induction it is clear that, if we can prove that ${}^N h_{(n)ab} = {}^X h_{(n)ab}$ holds on the characteristic hypersurface $N_1 \cup N_2$ for $a,b = 1,\ldots,4$ and $n = 1,\ldots,N$, then this equality will be valid also in the four-dimensional regions located in the future and the past of $N_1 \cap N_2$. This will prove [by performing the inverse coordinate transformation, $x'^a = f'^a(x^b,\lambda)$] that the originally given family of "approximately Ricci-flat metrics," Eq. (10), differs only by a term $\lambda^{N+1} k'_{ab}(x'^c,\lambda)$ from a family of exactly Ricci-flat metrics, namely the inverse coordinate transform of ${}^X g_{ab}(x^c,\lambda)$.

We have just shown that it suffices to prove that the full metric deviation on $N_1 \cup N_2$, $\left[{}^X g_{ab}(x^c,\lambda) - {}^N g_{ab}(x^c,\lambda) \right]_{N_1 \cup N_2}$ with $a,b = 1,\ldots,4$, tends to zero at least as λ^{N+1} when $\lambda \to 0$. Let us consider in detail what happens on N_1. For any covariant metric expressed in standard coordinates (as ${}^N g_{ab}$ and ${}^X g_{ab}$) there are only seven nonidentically vanishing components on N_1. Let us denote them as follows:

$$
g_{12} = :\alpha, \tag{18a}
$$

$$
g_{2A} = :\beta_A, \tag{18b}
$$

$$
g_{AB} = :\gamma_{AB} = \omega \tilde{\gamma}_{AB}, \tag{18c}
$$

$$
g_{22} = :\delta. \tag{18d}
$$

In Eq. (18c) we have decomposed γ_{AB} in the conformal factor ω and a reference conformal metric $\tilde{\gamma}_{AB}$ (which will be taken the same as the one appearing in the characteristic data). Let us also introduce the following abbreviations for quantities calculable in terms of the α's, β's, γ's, and δ's:

$$
\tilde{\theta} := \tfrac{1}{2} \tilde{\gamma}^{AB} D \tilde{\gamma}_{AB}, \tag{19a}
$$

$$
\tilde{\sigma}^B_A := \tfrac{1}{2} \tilde{\gamma}^{BC} D \tilde{\gamma}_{AC} - \tfrac{1}{2} \tilde{\theta} \delta^B_A, \tag{19b}
$$

$$
\dot{\gamma}^B_A := \gamma^{BC} D \gamma_{AC}, \tag{19c}
$$

$$\theta := \tfrac{1}{2}\dot{\tilde{\gamma}}^A_A \equiv \tfrac{1}{2}\gamma^{AB}D\gamma_{AB} = \tilde{\theta} + D\ln\omega, \tag{19d}$$

$$\gamma_A := \gamma^{BC}(\gamma_{AB,C} - \tfrac{1}{2}\gamma_{BC,A}), \tag{19e}$$

$$\omega_A := D\beta_A - \dot{\tilde{\gamma}}^B_A\beta_B + \tfrac{1}{2}\alpha\gamma_A. \tag{19f}$$

In Eqs. (19), $\tilde{\gamma}^{AB}$ (resp. γ^{AB}) denotes the inverse matrix of $\tilde{\gamma}_{AB}$ (resp. γ_{AB}), ln the natural logarithm, and the operator D denotes the differentiation along x^1 within N_1, i.e.,

$$D\varphi := \frac{\partial\varphi}{\partial x^1} \equiv \varphi_{,1} \equiv l(\varphi). \tag{20}$$

The short-hand notations (18) and (19) allow us to write down explicitly the analogs in the characteristic initial value problem of the well-known elliptic constraints of the space-like Cauchy problem. These characteristic constraints can be organized as a hierarchical system of ordinary differential equations relating the null hypersurface metric components (18) to the values on N_1 of some of the components of the four-dimensional Ricci tensor $R_{ab}[g]$. The obtention of these constraints was only sketched in the proof of Theorem 3 of Ref. 8. We have derived them explicitly for the purpose of proving our Theorem 2. For any, in general, non-Ricci flat, metric g_{ab} in standard coordinates we have identically along N_1:

$$E_\omega[D^2\omega, D\omega, \omega, \ldots] = -R_{11}, \tag{21a}$$

$$E_\alpha[D\alpha, \alpha, \ldots] = 0, \tag{21b}$$

$$E_A[D^2\beta_A, D\beta_A, \beta_A, \ldots] = \alpha R_{1A}, \tag{21c}$$

$$E_\delta[D^2\delta, D\delta, \delta, \ldots] = -\tfrac{1}{2}\alpha^2\gamma^{AB}R_{AB}, \tag{21d}$$

where

$$E_\omega := D^2\ln\omega + D\tilde{\theta} + \tfrac{1}{2}(D\ln\omega + \tilde{\theta})^2 + \tilde{\sigma}^B_A\tilde{\sigma}^A_B, \tag{22a}$$

$$E_\alpha := D\ln|\alpha| - \tfrac{1}{2}\theta, \tag{22b}$$

$$E_A := \left(D + \frac{\theta}{2}\right)\left[D\beta_A - \dot{\tilde{\gamma}}^B_A\beta_B + \frac{1}{2}\alpha\gamma_A\right] + \tfrac{1}{2}\alpha\dot{\tilde{\gamma}}^B_{A\|B} - \alpha\theta_{,A}, \tag{22c}$$

$$E_\delta := D\left(D - \frac{\theta}{2}\right)\delta - D \times [2\beta^A\omega_A - \tfrac{1}{2}\theta\beta^A\beta_A + \beta^A\beta_B\dot{\tilde{\gamma}}^B_A - \alpha\beta^A\gamma_A] + \alpha^2(\alpha^{-1}\omega^A)_{\|A} + \omega^A\omega_A - \tfrac{1}{2}\alpha^2R^{(2)}(\gamma). \tag{22d}$$

In Eqs. (22) we have introduced some operations and quantities associated with the two-dimensional Riemannian metric γ_{AB}: $\beta^A := \gamma^{AB}\beta_B$, $\omega^A := \gamma^{AB}\omega_B$, the double vertical bar denotes the Levi-Civita covariant derivative associated with γ_{AB}, and $R^{(2)}(\gamma) = \gamma^{AB}R^{(2)}_{AB}(\gamma)$ the curvature scalar of γ_{AB}, [$R^{(2)}(\gamma) = +2K$, where K is the Gauss curvature of the sections $x^1 = \text{const}$ of N_1].

As indicated by the notation of their left-hand sides, Eqs. (21) constitute a *hierarchical* system of ordinary differential equations in the following sense: (a) given $\tilde{\gamma}_{AB}$ on N_1, Eq. (21a) with (22a) indeed gives a second-order differential equation for ω, with "source" the value of R_{11} along N_1; (b) given $\tilde{\gamma}_{AB}$, R_{11} and a solution ω of the latter differential equation, Eq. (21b) with (22b) and (19d) gives a first-order differential equation for α; (c) given $\tilde{\gamma}_{AB}$, R_{11}, some solutions ω and α, as well as R_{1A} on N_1, Eqs. (21c) and (22c) give a second-order differential equation for β_A; and finally (d) given $\tilde{\gamma}_{AB}$, R_{11}, R_{1A}, some solutions ω, α, and β_A, as well as $\gamma^{AB}R_{AB}$ on N_1, Eqs. (21d), (22d) give a second-order differential equation for δ.

We wish to compare ${}^Xg_{ab}(x^c,\lambda)$ and ${}^Ng_{ab}(x^c,\lambda)$ on N_1, i.e., to compare $({}^Z\alpha, {}^Z\beta_A, {}^Z\gamma_{AB}, {}^Z\delta)$ for $Z = N$ and X. First, by definition [see Eq. (14a)] we know that ${}^N\gamma_{AB}$ and ${}^X\gamma_{AB}$ are conformal to the same reference metric $\tilde{\gamma}_{AB} := {}^N\gamma_{AB}$, which means that ${}^N\omega \equiv 1$ on N_1. On the other hand, ${}^X\omega$ is defined as *the* solution of Eq. (21a) with $\tilde{\gamma}_{AB} := {}^N\gamma_{AB}$ and ${}^XR_{11} = 0$, which starts off S (i.e., $x^1 = 0$) with the initial conditions $\omega(x^1 = 0) = 1$, $D\omega(x^1 = 0) = 0$ [see Eqs. (14b)]. In other words we are comparing the solutions of two ordinary differential equations,

$$D^2\ln({}^N\omega) + D\tilde{\theta} + \tfrac{1}{2}[D\ln({}^N\omega) + \tilde{\theta}]^2 + \tilde{\sigma}^B_A\tilde{\sigma}^A_B = -{}^NR_{11}, \tag{23a}$$

$$D^2\ln({}^X\omega) + D\tilde{\theta} + \tfrac{1}{2}[D\ln({}^X\omega) + \tilde{\theta}]^2 + \tilde{\sigma}^B_A\tilde{\sigma}^A_B = 0, \tag{23b}$$

with the same initial conditions at $x^1 = 0$. The coefficients of these two differential equations are smooth functions of x^1, x^A, and λ, and differ only (in the source) by the term $-{}^NR_{11}$, which we know, from Eq. (13), to be of the form $-\lambda^{N+1}S_{(N)11}(x^1,x^A,\lambda)$ with a smooth function $S_{(N)11}$. To simplify the reasoning we shall provisionally introduce a new parameter, say μ, to be identified later with λ^{N+1}. Then consider $u := (\omega, D\omega)$, and the solution of the first-order differential equation deduced from Eq. (21a) by replacing R_{11} by $\mu S_{11}(x^1,x^A,\lambda)$, say

$$\frac{\partial u}{\partial x^1} = F(u, x^1, x^A, \lambda, \mu), \tag{24}$$

which takes the value (1,0) at $x^1 = 0$. This solution, say $u = \varphi(x^1,x^A,\lambda,\mu)$, reduces to $({}^X\omega, {}^X\omega_{,1})$ when $\mu = 0$, and to $({}^N\omega, {}^N\omega_{,1})$ when $\mu = \lambda^{N+1}$. Moreover, as F and the initial conditions are smooth functions of all their arguments, one knows by standard theorems about parameter-dependent ordinary differential equations that φ is C^∞ jointly in the "independent variable" x^1, and the "parameters" (x^A,λ,μ). Therefore, we can write

$$\omega(x^1,x^A,\lambda,\mu) = {}^X\omega(x^1,x^A,\lambda) + \mu\hat{\omega}(x^1,x^A,\lambda,\mu), \tag{25a}$$

with $\hat{\omega}$ being C^∞ in all its arguments. Inserting (25a) into Eqs. (21b), (22b), and using Eq. (19d) yields

$$\frac{\partial}{\partial x^1}\ln|\alpha| = \frac{1}{2}\tilde{\theta} + \frac{1}{2}({}^X\omega + \mu\hat{\omega})^{-1}({}^X\omega_{,1} + \mu\hat{\omega}_{,1}). \tag{26}$$

The solution, say $\alpha(x^1,x^A,\lambda,\mu)$, of Eq. (26) with initial condition $\alpha(x^1 = 0) = -1$ (because of the definition of standard coordinates) reduces to ${}^X\alpha$ for $\mu = 0$ and to ${}^N\alpha$ for $\mu = \lambda^{N+1}$. We can again clearly see that α must be smooth in all its arguments, including μ, and that we can write

$$\alpha(x^1,x^A,\lambda,\mu) = {}^X\alpha(x^1,x^A,\lambda) + \mu\hat{\alpha}(x^1,x^A,\lambda,\mu), \quad (25b)$$

for some C^∞ function $\hat{\alpha}$.

We can proceed in the same manner for the next equation of the hierarchy, (21c), (22c), replacing R_{1A} by $\mu S_{(N)1A}(x^1,x^A,\lambda)$ [see Eq. (13)], and defining $\beta_A(x^1,x^A,\lambda,\mu)$ as the solution of Eq. (21c) with initial conditions $\beta_A(x^1=0)=0$ (because $g_{2A}\equiv 0$ on N_2 and therefore on $S=N_1\cap N_2$) and $D\beta_A(x^1=0) = {}^N g_{2A,1}(x^1=0)$ [see Eq. (14b)]. The insertion of Eqs. (25a) and (25b) into (21c), (22c) [using Eqs. (19c)–(19e) with $\gamma_{AB}=\omega(\mu)\times\tilde{\gamma}_{AB}$] leads to a differential equation for $\beta_A(x^1,\ldots,\mu)$ which: (i) depends smoothly on μ, and (ii) reduces to the one for ${}^X\beta_A$ when $\mu=0$ (and the one for ${}^N\beta_A$ when $\mu=\lambda^{N+1}$). As the initial conditions are also smooth in the parameters (and even independent of μ), standard theorems guarantee again the smoothness of the solution, so that one can write

$$\beta_A(x^1,x^A,\lambda,\mu) = {}^X\beta_A(x^1,x^A,\lambda) + \mu\hat{\beta}_A(x^1,x^A,\lambda,\mu), \quad (25c)$$

for some C^∞ functions $\hat{\beta}_A$. The same argument works for Eqs. (21d), (22d), replacing R_{AB} by $\mu S_{(N)AB}(x^1,x^A,\lambda)$ and using, besides the equations already mentioned, Eqs. (19f) and (25c) to check explicitly the smooth dependence in μ, and the reduction to the equation for ${}^X\delta$ when $\mu=0$. In that case the initial conditions are $\delta(x^1=0)=0$ (because $g_{22}\equiv 0$ on N_2), and $D\delta(x^1=0) = -\tilde{\theta}|_{N_2}$ (as deduced from the restriction to S of the harmonicity condition $\Gamma_2=0$; $\tilde{\theta}|_{N_2}$ denotes the reference "expansion" of N_2, i.e., the analog of (19a) computed along N_2, with D replaced by $\partial/\partial x^2$). Note that the various two-surface derivatives that are hidden in the three dots on the left-hand sides of Eqs. (21a)–(21d) (e.g., the ones included in the curvature scalar), as well as the other D derivatives, are harmless in the present reasoning because they act on already known (at each stage) smooth functions of x^1,x^A,λ, and μ. We then get also

$$\delta(x^1,x^A,\lambda,\mu) = {}^X\delta(x^1,x^A,\lambda) + \mu\hat{\delta}(x^1,x^A,\lambda,\mu), \quad (25d)$$

for some C^∞ function $\hat{\delta}$.

Replacing now μ by λ^{N+1} in Eqs. (25a)–(25d) we get

$$\text{on } N_1: {}^N g_{ab}(x^1,x^A,\lambda) = {}^X g_{ab}(x^1,x^A,\lambda) + \lambda^{N+1} k_{ab}(x^1,x^A,\lambda), \quad (27)$$

for $a,b=1,\ldots,4$, and for some smooth functions k_{ab}.

We can transpose the same reasoning for the constraints on N_2. The only differences, beyond exchanging the indices 1 and 2, are that the initial conditions for $g_{1A,2}$ are obtained from the ones for $g_{2A,1}$ by writing the restriction to S of the harmonicity condition $\Gamma_A=0$ [where we recall that Γ_a is defined by Eq. (15), and vanishes in standard coordinates]. Then the analog of (27) holds also on N_2. The combination of this just proven equality on $N_1\cup N_2$ of the first N coefficients of the Taylor expansions of ${}^N g(\lambda)$ and ${}^X g(\lambda)$ with the result obtained above on the uniqueness of the solution of the *reduced* perturbation hierarchy completes the proof of the first part of Theorem 3, the one concerning finite Taylor expansions.

Let us now start from a Ricci-flat background $g'_{(0)ab}(x'^c)$ and from an *infinite* sequence $h'_{(n)ab}(x'^c)$ satisfying the perturbation hierarchy (8). We can then construct a smooth one-parameter family of Lorentz metrics, by using the Theorem 1.2.6. of Ref. 20. This theorem generalizes Borel's theorem (given any sequence of numbers there exists a C^∞ function defined near the origin of the real line which has these numbers as successive derivatives at the origin) to sequences of smooth functions. This theorem guarantees (locally) the existence (and constructability) of a smooth λ-family ${}^\infty g'_{ab}(x'^c,\lambda)$ such that its value at $\lambda=0$ is $g'_{(0)ab}(x'^c)$, and its successive Taylor coefficients at $\lambda=0$ are the $h'_{(n)ab}(x'^c)$, for all $n\geqslant 1$. We can then use the same reasoning as above, starting now with ${}^\infty g'(\lambda)$ instead of ${}^N g'(\lambda)$ as "approximately Ricci-flat" metric. By a (locally smooth) λ-dependent coordinate transformation we can introduce standard coordinates. Then we use $[{}^\infty g_{AB}]_{N_1\cup N_2}$ and $[{}^\infty g_{2A,1}]_S$ as characteristic data to define a family of exactly Ricci-flat metrics, in standard coordinates, say ${}^X g_{ab}(x^c,\lambda)$. The comparison between the two families is done as above, ${}^\infty R_{ab}(x^c,\lambda) = \lambda^{N+1} S_{(N)ab}(x^c,\lambda)$ holding for any given value of N. This shows then that ${}^\infty g(\lambda)$ and ${}^X g(\lambda)$ have the same infinite sequence of Taylor coefficients at $\lambda=0$ (both in standard coordinates, and in the original coordinate system). □

Note that, in a general C^∞ setting, there are many exact solutions giving rise to a given sequence of Taylor coefficients. Only in the case where the formal series in powers of λ that correspond to the characteristic data $[{}^\infty g_{AB}]_{N_1\cup N_2}$ and $[{}^\infty g_{2A,1}]_S$ converge can we single out a preferred C^∞ family of exact solutions.

Let us remark that the proof we gave of the local reliability of Einstein's vacuum field equations is essentially based on two broad facts: (i) the reduction, in some gauge, of the evolution equations to a system of quasilinear wave equations for some collection of fields, say ϕ (in our case the ten g_{ab}'s in harmonic coordinates), and (ii) the fact that the characteristic initial value problem leads to a hierarchical set of ordinary differential equations for determining the full characteristic data for the "reduced" field equations (i.e., the values of all the ϕ's on $N_1\cup N_2$) from some "free" characteristic data, say χ (in our case, essentially the conformal two-metric $\tilde{\gamma}_{AB}$). The essential structure used in the proof above of this hierarchical set of ordinary differential equations has been that it was a smooth function of the hypersurface derivatives of the ϕ's and the χ's up to some finite order, and of any possible source term in the original field equations.

Let us consider now the coupled Einstein–Yang–Mills system (see Theorem 2 above). It belongs to the just described (ϕ,χ) class of systems to which our method applies, if we take $\phi=(g_{ab},\mathbf{A}_a)$ in standard gauge (see Definition 2 above), and for χ the data of Theorem 2. We find that the Einstein–Yang–Mills equations in standard gauge, considered along the null hypersurface N_1, imply the following hierarchical set of ordinary differential equations:

$$E'_\omega[D^2\omega,D\omega,\omega,\ldots]:=E_\omega+k\omega^{-1}\tilde{\gamma}^{AB}\mathbf{K}_A\cdot\mathbf{K}_B=0, \quad (28a)$$

$$E_\alpha[D\alpha,\alpha,\ldots]=0, \quad (28b)$$

$$\mathbf{E}_\sigma[D\boldsymbol{\sigma},\boldsymbol{\sigma},\ldots]:=(D+\theta)\boldsymbol{\sigma}+\mathbf{K}^B{}_{\|B}+[\mathbf{A}_B,\mathbf{K}^B]=0, \quad (28c)$$

$$E'_A[D^2\beta_A,D\beta_A,\beta_A,\ldots]:$$
$$=E_A+k\alpha[\mathbf{K}_A\cdot\boldsymbol{\sigma}+\mathbf{F}_{AB}\cdot\mathbf{K}^B]=0, \quad (28d)$$

$$E'_\delta[D^2\delta,D\delta,\delta,\ldots]:$$
$$=E_\delta+\tfrac{1}{2}k\alpha^2[\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}+\tfrac{1}{2}\gamma^{AA'}\gamma^{BB'}\mathbf{F}_{AB}\cdot\mathbf{F}_{A'B'}]=0, \quad (28e)$$

$$\mathbf{E}_{\mathbf{A}_2}[D\mathbf{A}_2,\ldots]:=D\mathbf{A}_2-\beta^B D\mathbf{A}_B$$
$$+\tfrac{1}{2}\alpha\gamma^{AB}\mathbf{A}_{B,A}+\tfrac{1}{2}\alpha\boldsymbol{\sigma}=0, \quad (28f)$$

where $\mathbf{K}_B$ denotes $-\partial_1\mathbf{A}_B$ (i.e., $\mathbf{F}_{B1}$ in standard gauge) and $\mathbf{K}^B:=\gamma^{BC}\mathbf{K}_C$. Along N_2 a corresponding set of equations must also hold. The initial conditions on S for these differential equations have been given in the proof of Theorem 2 above. When one considers (as needed in the proof of reliability) inhomogeneous Einstein–Yang–Mills systems,

$$R_{ab}-k\tau_{ab}=S_{ab},$$
$$\mathbf{Y}_a=\mathbf{J}_a,$$

but still works in standard gauge, Eqs. (28) acquire the following respective source terms:

$$-S_{11},0,-\mathbf{J}_1,\alpha S_{1A},-\tfrac{1}{2}\alpha^2\gamma^{AB}S_{AB},0.$$

This makes it clear that our method of proof applies. Therefore, one can conclude that Theorem 3 generalizes completely to the Einstein–Yang–Mills equations.

Finally, the treatment of the characteristic initial value problem for the Einstein–Euler system (general relativistic perfect fluid) in Ref. 8 shows that our method can also be applied to prove the local reliability of perturbation expansions for the coupled gravitation-perfect fluid system. However, this local result is valid only in a connected domain where $\rho+p(\rho)>0$, i.e., inside one gravitating fluid, and, therefore it provides no mathematical justification to the use, say, of post-Minkowskian perturbation series to represent the gravitational field generated by finite bodies. What would be needed for this problem is, first of all, an existence theorem for solutions describing bodies of finite extent. In this respect it is amusing to note that, if the recently found "particlelike" solutions of the Einstein–Yang–Mills equations[21] turn out to be stable, they might be of use in modeling an "N-body system" for which, as we just showed, a reliability result exists.

V. SMOOTH ONE-PARAMETER FAMILIES OF SEMIGLOBAL PAST-STATIONARY SPACE-TIMES ADMITTING A PIECE OF $\mathscr{T}$ WITH RADIATION

Up to now we have considered only the question of the *local* reliability of perturbation theory. Our positive answer to this question allows one to justify the use of perturbation expansions to approximate, say, vacuum gravitational fields over *compact* space-time domains. However, the algorithm developed by Blanchet and Damour[2] was intended to approximate generic vacuum gravitational fields all over a noncompact "weak-field zone outside the source." More precisely, their algorithm assumes the existence of, what can be called, "semiglobal past-stationary radiative vacuum space-times" (for short, "semiglobal space-times") i.e., solutions of the vacuum Einstein equations over a manifold homeomorphic to $\mathscr{R}^4$ minus a timelike cylinder, which are stationary before some time, and which admit (at least a piece of) a regular future null infinity ($\mathscr{T}^+$) with radiation. In subsequent papers[22] they used their post-Minkowskian algorithm to study the structure of the gravitational radiation emitted by isolated material sources. The question therefore naturally arises whether our result of local reliability can be extended to one of semiglobal reliability, which would give a mathematical justification to such perturbation approaches. By combining the method we used in Sec. IV with theorems of Friedrich[12] on the regularization of the conformal Einstein equations we shall show that this is the case. More precisely we are going to prove: (i) the existence of semiglobal past-stationary solutions of the vacuum Einstein equations admitting a piece of $\mathscr{T}$, and (ii) the possibility to construct smooth one-parameter families of such semiglobal solutions whose Taylor coefficients in the λ expansion are of the "multipolar post-Minkowskian type" studied in Refs. 2 and 22. The generalization of this construction to the Einstein–Yang–Mills system is briefly discussed at the end of this section.

To prove the existence of semiglobal past-stationary radiative vacuum space-times let us start by giving ourselves a semiglobal *stationary* solution of the vacuum Einstein equations which is asymptotically flat, say ${}^s g$. Choose an asymptotically flat spacelike hypersurface C^3 (homeomorphic to $\mathscr{R}^3$ minus a ball) such that ${}^s g$ is defined on the manifold $C^3\times\mathscr{R}$ (in the static case we would naturally take one of the preferred spacelike hypersurfaces orthogonal to the Killing vector). Select on C^3 a spacelike two-surface S (of spherical topology) such that the outgoing future-directed null geodesics issued from S generate a smooth null hypersurface, N_{out}, up to $\mathscr{T}^+$ (no caustics). Denote by N_{in} the null hypersurface generated locally by the ingoing future-directed null geodesics issued from S [see Fig. 1(a)]. We shall use the two null hypersurfaces[23] N_{out}, N_{in} to pose a characteristic initial value problem (using, say, two patches of standard coordinates to cover S and its neighborhood). We consider a smooth one-parameter (or several-parameter) family of initial data on $(S, N_{\text{out}}, N_{\text{in}})$ such that: (i) they coincide on S and N_{out} with the data for ${}^s g$ for all λ's; (ii) they reduce when $\lambda=0$ to the data for ${}^s g$; (iii) when $\lambda\neq 0$ the data on N_{in} differ (smoothly) from the data for ${}^s g$ only on the part of N_{in} which is in the future of a null hypersurface N'_{out} obtained by Lie dragging N_{out} some finite time in the future along the timelike Killing vector defining the stationarity of ${}^s g$ and extending it inwards down to N_{in} [see Fig. 1(a)]. Rendall's results recalled in Sec. III above guarantee the existence and uniqueness of a smooth family of solutions, say $g_D(\lambda)$, generated by such data only in some local four-dimensional domain, say D^4, which is a neighborhood of S intersected with

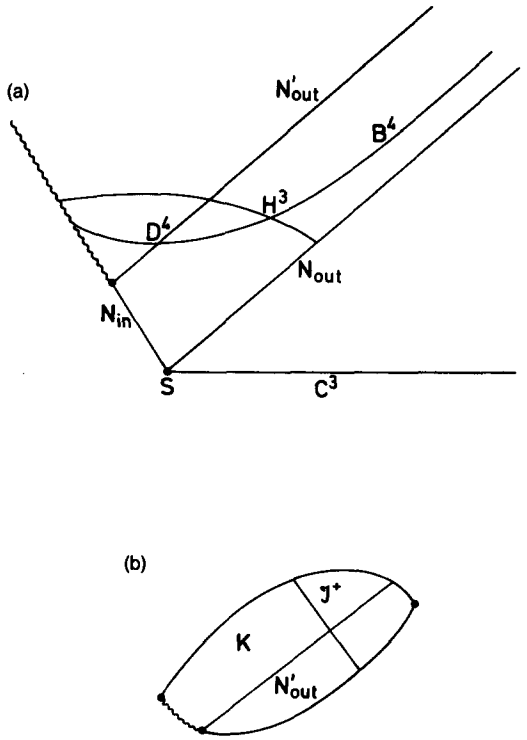

FIG. 1. (a) Construction of hyperboloidal data in physical space-time by piecing together a local characteristic initial value problem and a stationary solution. (b) Evolution of the hyperboloidal data in an extended conformal picture.

the future of S. Let us now introduce the infinite four-dimensional domain B^4 defined as the union of the local domain D^4 with the domain sandwiched between N_{out} and N'_{out} (and bounded inwardly by N_{in}). By our choice of data, it is clear that we can define on B^4 a smooth family of solutions of Einstein's vacuum field equations, say $g_B(\lambda)$, as being $g_D(\lambda)$ on D^4 and ${}^5g$ on $B^4 - D^4$. In the pseudo-Riemannian manifold $(B^4, g_B(\lambda))$ we can select a smooth spacelike hypersurface, say H^3, which starts off in the "nonstationary" part of B^4 (i.e., the future of N'_{out}) and then extends out to $\mathcal{I}^+$ through the "stationary" part of B^4 in a smooth asymptotically null manner (such H^3's are called "hyperboloids").

We can now use the theorems of Friedrich[12] about the regularization of the conformal Einstein vacuum equations to extend the nonstationary character of the metric out to infinity. By construction the metric $g_B(\lambda)$ induces on the asymptotically null spacelike hypersurface H^3 data, say $(h(\lambda), k(\lambda))$, that satisfy the "hyperboloidal constraints" of Ref. 12. Now, when $\lambda = 0$ the data $(h(0), k(0))$ correspond (by our choice above of local characteristic data) to the stationary metric ${}^5g$, and therefore define uniquely ${}^5g$ on the full domain of dependence of H^3. But such an asymptotically flat stationary metric is analytic at future null infinity, and admits a (unique) analytic extension through $\mathcal{I}^+$ (this was shown explicitly for the Schwarzschild solution in Ref. 24, and is discussed for the general case in the Appendix). Placing ourselves in such an analytically extended conformal picture (in which $\mathcal{I}^+$ is brought down to a finite "distance"), Fig. 1(b), we see that we have shown the existence of a smooth family of Cauchy data for the conformal vacuum equations that satisfy the constraints for all λ's, and that determine when $\lambda = 0$ a known solution of Friedrich's conformal evolution equations in some domain K (which is compact in this conformal picture, but which extends beyond null infinity). As Friedrich's evolution equations constitute a symmetric hyperbolic quasilinear system we can use the general result of Hamilton[7] of (C^∞) stability (under variation of the data) of the Cauchy development of the data in a compact domain K having a spacelike future boundary. Therefore, for λ small enough, we will have a smooth family of conformal metrics containing smooth (null) hypersurfaces on which the conformal factor vanishes.

Going back to the physical picture, we conclude that we have proven (for λ small enough, i.e., for small enough deviations about some stationary metric) the existence of smooth families of semiglobal nonstationary solutions of the vacuum Einstein equations that are stationary before some retarded time, and which admit a smooth piece of future null infinity, up to some (later) retarded time. Note that our class of solutions is rather general as it contains (for each λ) two arbitrary functions of three variables. It is also interesting to note that, after having constructed our solutions by means of a characteristic initial value problem, we can also consider the data they induce on a usual spacelike Cauchy surface (homeomorphic to $\mathcal{R}^3$ minus a ball). As these Cauchy data (first and second fundamental forms) belong to a stationary space-time outside some two surface they clearly satisfy the asymptotic spatial fall-off conditions used in the recent work of Christodoulou and Klainerman.[25] If we assume that their result (proven for Cauchy surfaces homeomorphic to $\mathcal{R}^3$) holds true also for (small enough) data considered on a Cauchy surface homeomorphic to $\mathcal{R}^3$ minus a ball, we can say that our result proves the existence of a subclass of Cauchy data which evolve into a (piece of a) smooth $\mathcal{I}$. The existence of such "good" data is not clear from their results, as the estimates they get for the fall off of the gravitational field at null infinity violate the "peeling property," and would therefore be incompatible with even a C^3 conformal structure at $\mathcal{I}$ if they were sharp. An indication of how both types of results can be reconciled comes from perturbation calculations. Indeed, some perturbative results[26] get a smooth $\mathcal{I}$ for generic semiglobal past-stationary (approximate) space-times, but find, when a limit is taken that allows the space-time to have been always nonstationary, that the smoothness of $\mathcal{I}$ can be destroyed, and that the peeling property may not hold (neither at $\mathcal{I}^-$ nor at $\mathcal{I}^+$). These calculations indicate also that the past-stationarity of these semiglobal approximate space-times is a sufficient but not necessary condition for the smoothness of $\mathcal{I}$. What seems needed is just a sufficiently fast approach to stationarity when going back in the past. In terms of Cauchy data, this would correspond to data that never belong, near spatial infinity, to a stationary space-time, but which, in some sense, tend fast enough to "stationary data" to preserve the smoothness of $\mathcal{I}$. (We are assuming here that the global time asymmetry, "no incoming radiation condition," which is built in most of the perturbation calculations is not crucial compared to the spatial fall-off). This suggests the interest-

ing mathematical question of trying to characterize such "asymptotically stationary" data leading to a smooth $\mathscr{T}$ among the general class of data which, probably (because of the singular conformal structure at spatial infinity, and of the existing exact[25] and perturbative[26] results), lead generically to a violation of peeling.

In the above construction we have used the parameter dependence only to simplify our need to deviate slightly from a stationary solution. However, we can also put a parameter dependence in the data that define the stationary solution. In particular we can, for instance, replace the mass M by λM in the characteristic data for the Schwarzschild solution, and add, on N_{in}, nonstationary data that have also λ in factor and which contain only a finite number of multipoles (starting smoothly off zero at some retarded time corresponding to N'_{out}). Such data will generate a smooth family of semiglobal exact solutions whose λ expansion will be of the type of the "multipolar post-Minkowskian" expansions studied in Refs 2 and 22. Thereby we have extended our result of local reliability of perturbation expansions to one of semiglobal reliability (including at future null infinity) for such "multipolar post-Minkowskian" expansions.

Finally, we can straightforwardly generalize all the steps of our construction to the Einstein–Yang–Mills case. The basic ingredients we need are available: they are the existence and uniqueness of C^∞ solutions generated by C^∞ characteristic data (Theorem 2 above) and the possibility to regularize the conformal Einstein–Yang–Mills equations.[27] As above, this proves the existence of a general class of semiglobal past-stationary radiative Einstein–Yang–Mills (and in particular Einstein–Maxwell) solutions admitting a C^∞ conformal structure on a piece of $\mathscr{T}$, and the possibility to construct smooth multipolar-post-Minkowskian-type families of such solutions.

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APPENDIX: ANALYTIC EXTENSION THROUGH $\mathscr{T}$ OF STATIONARY VACUUM METRICS

There are various ways, starting from the theorem of Beig and Simon,[28] to show that, for a stationary asymptotically flat solution of the vacuum Einstein equations, there exists a chart (u,r,θ,φ) such that the metric is conformal to a metric analytic in $\tilde{r} := 1/r$ near $\tilde{r} = 0$. In general, such a chart will not be harmonic. If we wish, we can however assume that the conditions of harmonicity are satisfied up to some finite order. If we assume that the mass does not vanish, and that the mass dipole is transformed to zero we have a metric of the form[29]

$$
\begin{aligned}
ds^2 = & -\left(1 - \frac{2M}{r} + \frac{2M^2}{r^2} + \frac{F}{r^3}\right) dt^2 \\
& - \left(4\epsilon_{\alpha\beta\gamma} \frac{S^\beta z^\gamma}{r^3} + \frac{F_\alpha}{r^3}\right) dt\, dz^\alpha \\
& + \left[\delta_{\alpha\beta}\left(1 + \frac{2M}{r} + \frac{3}{2}\frac{M^2}{r^2}\right) + \frac{F_{\alpha\beta}}{r^3}\right] dz^\alpha\, dz^\beta,
\end{aligned}
$$

where $r^2 := \delta_{\alpha\beta} z^\alpha z^\beta$; $\alpha,\beta = 1,2,3$. Note that the freedom of making spatial transformations was used for having a spatial metric which is conformally flat up to the order $O(1/r^3)$. The functions F, F_α, $F_{\alpha\beta}$ into which we have collected the higher-order terms are analytic in $1/r$ and in the angular coordinates, $(\theta,\varphi) = (\phi^A)$; $A = 3,4$. Going to standard polar coordinates one checks easily that all the terms of the conformal metric $d\tilde{s}^2 := r^{-2}\, ds^2$ are analytic in $\tilde{r} := 1/r$ near $\tilde{r} = 0$, in the $(t,\tilde{r},\theta,\varphi)$ chart, except for the term proportional to $d\tilde{r}^2$. To take care of that term we must transform the time coordinate. The dangerous terms are contained in

$$
\begin{aligned}
ds'^2 &= -A^2(r)dt^2 + B^2(r)dr^2 \\
&= -A^2(dt - (B/A)dr)(dt + (B/A)dr),
\end{aligned}
$$

where

$$A^2 = 1 - 2M/r + 2M^2/r^2,$$

$$B^2 = 1 + \frac{2M}{r} + \frac{3}{2}\frac{M^2}{r^2}.$$

If we define a new time coordinate by

$$u = t - \int \frac{B(r)}{A(r)}\, dr,$$

we obtain

$$
\begin{aligned}
ds'^2 &= -A^2\, du(du + (2B/A)dr) \\
&= -A^2\, du^2 - 2AB\, du\, dr.
\end{aligned}
$$

We can now check that $d\tilde{s}^2 = r^{-2}\, ds^2$ is analytic in $\tilde{r}$, at $\tilde{r} = 0$, in the $(u,\tilde{r},\theta,\varphi)$ chart. The hypersurface $\tilde{r} = 0$ is easily seen to be a null hypersurface, with topology $\mathscr{R} \times S^2$.

[1] D. Christodoulou and B. G. Schmidt, Commun. Math. Phys. **68**, 275 (1979).

[2] L. Blanchet and T. Damour, Phil. Trans. R. Soc. London Ser. A **320**, 379 (1986).

[3] Our conventions and notation are the following: signature $- + + +$; $a,b,...,i,j,... = 1,2,3,4$; $A,B,... = 3,4$; $\alpha,\beta,... =$ three spatial indices when needed; Ricci tensor $R_{ab} = \Gamma^c_{ab,c} - \Gamma^c_{ac,b} + \Gamma\Gamma$.

[4] Y. Choquet-Bruhat and J. W. York, Jr., "The Cauchy Problem," in *General Relativity and Gravitation*, edited by A. Held (Plenum, New York, 1980), Vol. 1, pp. 99–172; J. M. Arms, J. E. Marsden, and V. Moncrief, Ann. Phys. **144**, 81 (1982).

[5] Defining the differentiability class of a curve of solutions of a nonlinear system of partial differential equations requires specifying the functional spaces one is working with: e.g., a Banach space of C^k functions on a

compact set K, or some Sobolev space over K. In the present paper, it will be sufficient to define a C^∞ curve $g(\lambda)$ as a one-parameter family of metrics such that, in some local chart, the metric coefficients $g_{ab}(x^c,\lambda)$ are jointly C^∞ in x^c and λ. The derivatives in the Banach sense reduce then to usual partial derivatives with respect to λ.

[6] Y. Choquet-Bruhat, Uspekhi Mat. Nauk. **29**, 314 (1976).

[7] R. S. Hamilton, Bull. (New Series) Am. Math. Soc. **7**, 65 (1982).

[8] A. Rendall, Proc. R. Soc. London Ser. A **427**, 221 (1990).

[9] This terminology can be accordingly modified if one wishes to consider solutions of the perturbation hierarchy truncated at some finite order, and, correspondingly, curves of solutions of finite differentiability (e.g., "linearization stability" is equivalent to "first-order reliability"). Note that our use of the word "reliability" is different, and in our opinion, more appropriate than the one of Geroch and Lindblom [J. Math. Phys. **26**, 2581 (1985)] which would be better called, say, "extendability."

[10] The seemingly contradictory results of Geroch and Lindblom (quoted in Ref. 9) do not conflict with ours, because they consider the perturbation equations of general relativity *constrained* by symmetry requirements.

[11] J. Ehlers, in *Grundlagenprobleme der Modernen Physik*, edited by J. Nitsch *et al.* (Bibl. Inst., Mannheim, 1981), pp. 65–84; M. Lottermoser, Ph.D. dissertation, Munich University, 1988 (unpublished).

[12] H. Friedrich, Commun. Math. Phys. **91**, 445 (1983); **107**, 587 (1986).

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[15] The future (resp. past) of S is defined as the set of events that can be connected to a point of S by a future-directed (resp. past-directed) nonspacelike curve. The future of S is also the intersection of the futures of N_1 and N_2. In standard coordinates, if the null vector $\vec{l} = \partial/\partial x^1$ is chosen to be future directed (which implies, because of $[\vec{l}\cdot\vec{n}]_S = -1$ and of the signature $(-+++)$, that $\vec{n} = \partial/\partial x^2$ is also future directed), the future (resp. past) of S corresponds to $x^1 \geqslant 0$ and $x^2 \geqslant 0$ (resp. $x^1 \leqslant 0$ and $x^2 \leqslant 0$).

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[22] L. Blanchet, Proc. R. Soc. London Ser. A **409**, 383 (1987); L. Blanchet and T. Damour, Ann. Inst. H. Poincaré (Physique théorique) **50**, 377 (1989).

[23] Note that in the following "hypersurface" means in fact "half-hypersurface" as we are interested in constructing solutions that are stationary in the past, and start off being radiative only in the future of S.

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[27] H. Friedrich, J. Diff. Geom. (in press).

[28] R. Beig and W. Simon, Proc. R. Soc. London Ser. A **376**, 333 (1981).

[29] For more details about these matters see a forthcoming book on the asymptotics of space-times by A. Ashtekar and B. G. Schmidt.

Exact model for a relativistic star

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Assuming that the physical three-space in a relativistic superdense star has the geometry of a three-spheroid, a static spherically symmetric model based on an analytic closed-form solution of Einstein's field equations is presented. Assuming the density of the order of 2×10^{14} g cm^{-3}, estimates of the total mass and size of the stars of the model are obtained for various values of a density-variation parameter that is suitably defined. The total mass and the boundary radius of each of these models are of the order of the mass and size of a neutron star.

I. INTRODUCTION

The models for relativistic spherical stars are usually constructed by integrating numerically the appropriate set of Einstein's field equations on the basis of an *a priori* furnished equation of state of its matter content. The precise nature of the behavior of matter in the central core regions of superdense stars like neutron stars being not known with certainty, one does not have reliable information about the equation of state for the matter content of such stars and one is led to make assumptions of a very general nature. However, the self-interaction of the gravitational field as reflected in the nonlinearity of Einstein's field equations, makes it difficult to obtain simple exact solutions useful for constructing models for relativistic stars. This problem has been considered by several authors.[1-7]

According to general relativity theory, the geometry of the physical space is governed by the matter-energy content of the space, which introduces curvatures in the acompanying space-time. The physical three-space of the Schwarzschild interior solution, representing the gravitational field in the interior of a cold star filled with a uniform distribution of matter in equilibrium, is curved up into a three-spherical space whose radius R is directly linked with the density of matter content of the star. Following this observation Vaidya and Tikekar[8] have shown that space-times whose associated physical three-spaces obtained as $t=$ const sections have geometry of a three-spheroid are useful in developing relativistic models for superdense spherical condensations of matter in equilibrium such as neutron stars. Only a few of the large number of closed-form solutions of Einstein's field equations for static spherical destributions of matter admit such possibilities. Accordingly, it is important to have exact solutions representing static fluid spheres that may serve as easily surveyable models for relativistic stars. The particular class of the superdense-star model of Vaidya and Tikekar[8] is found to permit higher values of maximum mass for a neutron star than the values permitted according to the nonnuclear analysis of Rhodes and Ruffini.[9] Knutsen[10] has discussed various physical properties of the Vaidya–Tikekar model and has shown that it is stable with respect to infinitesimal radial pulsations.

In this paper, after a brief discussion of the distinctive features of the space-times whose associated physical three-spaces have the geometry of a three-spheroid in Sec. I, we have obtained in Sec. II the relations governing the physical variables of equilibrium configurations of spherical distributions of matter, assuming that the background space-time has the above geometry. An exact solution of Einstein's field equations obtained in Sec. III, in this setup, is used to develop in subsequent sections a relativistic model for a superdense star. Specifying the matter density on the boundary surface of the configuration to be 2×10^{14} g cm^{-3}, the value given by Rees *et al.*,[11] for the surface density of matter for a neutron star, estimates of the total mass and size of the stars of the model are obtained for various values of a suitably introduced density-variation parameter. These estimates together with other relevant quantities are presented in Table I.

These values show that the closed-form solution presented here leads to a class of physically viable static models for relativistic stars. An important feature of this class of models is that if the matter content of star of the model complies with the requirement $\rho - 3p/c^2 > 0$ inherent in the strong energy conditions, the maximum permissible mass is

TABLE I. Masses and equilibrium radii corresponding to $\rho_a = 2.0\times 10^{14}$ g cm^{-3}, for the class of relativistic star models.

Ser. No.	λ	R(km)	a(km)	m(km)	$M/M_\odot$[a]	A	B
1	0.95	78.16	5.23	0.09	0.06	−1.93	1.97
2	0.9	76.08	7.36	0.26	0.18	−1.87	2.06
3	0.85	73.93	8.97	0.48	0.33	−1.79	2.14
4	0.80	71.73	10.31	0.75	0.51	−1.72	2.23
5	0.75	69.45	11.47	1.05	0.71	−1.64	2.31
6	0.70	67.09	12.49	1.39	0.94	−1.55	2.39
7	0.65	64.65	13.41	1.77	1.20	−1.46	2.48
8	0.60	62.12	14.24	2.19	1.49	−1.36	2.55
9	0.55	59.47	14.99	2.64	1.79	−1.25	2.63
10	0.50	56.70	15.68	3.12	2.12	−1.14	2.70
11	0.45	53.79	16.30	3.64	2.47	−1.01	2.76
12	0.40	50.72	16.86	4.20	2.85	−0.87	2.80
13	0.35	47.44	17.35	4.79	3.24	−0.71	2.83
14	0.30	43.92	17.78	5.43	3.68	−0.53	2.82
15	0.25	40.10	18.13	6.10	4.14	−0.33	2.76
16	0.20	35.86	18.39	6.81	4.62	−0.08	2.59
17	0.15	31.06	18.54	7.56	5.12	0.21	2.23
18	0.10	25.36	18.53	8.36	5.67	0.55	1.34

[a] Note: $M = mc^2/G$, $M_\odot$ = mass of the Sun.

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close to the limit imposed by the analysis of Rhodes and Ruffini.[9] Higher masses are permissible if the above condition is relaxed.

II. STATIC SPHEROIDAL SPACE-TIME

A three-spheroid, immersed in the four-dimensional Euclidean space with metric

$$d\sigma^2 = dx^2 + dy^2 + dz^2 + dw^2, \tag{2.1}$$

will have the Cartesian equation

$$(x^2 + y^2 + z^2)/R^2 + w^2/b^2 = 1. \tag{2.2}$$

The sections $w = \text{const}$ of the three-spheroid are concentric spheres, while sections $x = \text{const}$, $y = \text{const}$, and $z = \text{const}$ represent, respectively, systems of confocal ellipsoids.

The parametrization

$$\begin{aligned} x &= R \sin\alpha \sin\theta \cos\phi, \\ y &= R \sin\alpha \sin\theta \sin\phi, \\ z &= R \sin\alpha \cos\theta, \\ w &= b \cos\alpha, \end{aligned} \tag{2.3}$$

of the three-spheroid leads to

$$\begin{aligned} d\sigma^2 = {} & (R^2 \cos^2\alpha + b^2 \sin^2\alpha) d\alpha^2 \\ & + R^2 \sin^2\alpha (d\theta^2 + \sin^2\theta\, d\phi^2), \end{aligned} \tag{2.4}$$

as the metric on the three-spheroid. Introducing a new space variable

$$r = R \sin\alpha, \tag{2.5}$$

the metric $d\sigma^2$ on the three-spheroid can be cast into the form

$$\begin{aligned} d\sigma^2 = {} & [1 - K(r^2/R^2)](1 - r^2/R^2)^{-1} dr^2 \\ & + r^2 (d\theta^2 + \sin^2\theta\, d\phi)^2, \end{aligned} \tag{2.6}$$

where

$$K = 1 - b^2/R^2. \tag{2.7}$$

It is evident that a spheroidal three-space is essentially spherically symmetric. Its geometry is governed by two curvature parameters R and K. The metric (2.6) is regular and positive definite at all points $r < R$ for $K < 1$.

In the case $K = 1$, the spheroidal three-space degenerates into a flat three-space and in the case $K = 0$, it becomes spherical. The static spherically symmetric space-time of the metric,

$$\begin{aligned} ds^2 = {} & -[1 - K(r^2/R^2)](1 - r^2/R^2)^{-1} dr^2 - r^2 d\theta^2 \\ & - r^2 \sin^2\theta\, d\phi^2 + e^{\nu(r)} dt^2, \end{aligned} \tag{2.8}$$

has its associated three space, obtained as hypersurface $t = \text{const}$, a three-spheroidal space. The metric (2.8) with $K = 0$ and $e^{\nu(r)} = [A + B(1 - r^2/R^2)^{1/2}]^2$ is the metric of the Schwarzschild interior solution that is used to construct relativistic model for a cold, spherical star filled with uniform distribution of matter in equilibrium.

III. MATTER DISTRIBUTION ON SPHERIODAL SPACE-TIME

We consider spherical distributions of matter in the form of a perfect fluid represented by the space-time metric (2.8) when $K < 1$ and $K \neq 0$, i.e., when the physical three-space in (2.8) is spheroidal and not spherical or flat.

The energy-momentum tensor for a perfect fluid is given by

$$T_{ij} = (\rho + p/c^2) u_i u_j - (p/c^2) g_{ij}, \tag{3.1}$$

where ρ and p, respectively, denote matter density and fluid pressure and u^i represents the unit, four-velocity field of the fluid. For equilibrium configurations with background space-time metric (2.8)

$$u^i = (0,0,0,e^{-\nu/2}). \tag{3.2}$$

Einstein's field equations,

$$R_{ij} - \tfrac{1}{2} R g_{ij} = -(8\pi G/c^2) T_{ij}, \tag{3.3}$$

lead to

$$\frac{8\pi G}{c^2}\rho = \frac{3(1-K)}{R^2} \frac{[1 - (K/3)(r^2/R^2)]}{[1 - K(r^2/R^2)]^2}, \tag{3.4}$$

$$\frac{8\pi G}{c^4} p = \left(\frac{\nu'}{r} + \frac{1}{r^2}\right)\left(1 - \frac{r^2}{R^2}\right)\left(1 - K\frac{r^2}{R^2}\right)^{-1} - \frac{1}{r^2}, \tag{3.5}$$

as the relations determining matter density ρ and fluid pressure p in the distribution, together with the consistency condition implied in the isotropy condition $T_1^1 = T_2^2$, viz,

$$\begin{aligned} & \left(1 - \frac{r^2}{R^2}\right)\left(1 - K\frac{r^2}{R^2}\right)\left(\nu'' + \frac{\nu'^2}{2} - \frac{\nu'}{r}\right) \\ & \quad - \frac{2(1-K)r}{R^2}\left(\frac{\nu'}{2} + \frac{1}{r}\right) \\ & \quad + \frac{2(1-K)}{R^2}\left(1 - K\frac{r^2}{R^2}\right) = 0. \end{aligned} \tag{3.6}$$

Here, and in what follows, a prime indicates a differentiation with respect to r.

In this approach, the usual equation of state of matter is replaced by the geometrical requirement that the physical three-space of the distribution be spheroidal. In the Schwarzschild interior solution $K = 0$ and the matter density is linked directly with the geometric parameter R—the radius of the spherical three-space. In the present case, the geometric parameter R and K completely determine the matter density at all points of the distribution.

Let

$$m(r) = \frac{4\pi G}{c^2} \int_0^r \xi^2 \rho(\xi) d\xi \tag{3.7}$$

represent the total mass content of the distribution within the spherical region of radius r. The expression (3.4) for matter density gives

$$m(r) = \frac{1}{2} \frac{r^2}{R^2} \frac{(1-K)r}{1 - K(r^2/R^2)}. \tag{3.8}$$

The condition

$$\frac{1}{c^2}\frac{dp}{dr} = -\frac{(\rho + p/c^2)}{r^2}\left(\frac{[m(r) + (4\pi G p/c^4) r^3]}{1 - 2m(r)/r}\right), \tag{3.9}$$

which ensures the hydrostatic equilibrium of spherically symmetric distributions of matter, contained in the field equations (3.4), (3.5), and (3.6), can be written in the form

$$\frac{1}{c^2}\frac{dp}{dr} = -\frac{1-K(r^2/R^2)}{(1-r^2/R^2)}\left(\frac{4\pi G p r}{c^4} + \frac{(1-K)r}{2R^2[1-K(r^2/R^2)]}\right)\left(\rho + \frac{p}{c^2}\right). \quad (3.10)$$

The matter density ρ as given by Eq. (3.4) is positive throughout the distribution. Accordingly, we observe from (3.10) that if $p(r) > 0$ then the pressure gradient is negative at r and pressure will be decreasing radially outward.

IV. A SOLUTION OF FIELD EQUATIONS

The linear differential equation (3.6) can be expressed in the convenient form

$$(1 - K + Kz^2)\frac{d^2\psi}{dz^2} - Kz\frac{d\psi}{dz} + K(K-1)\psi = 0, \quad (4.1)$$

by adopting ψ and z defined by

$$\psi = e^{\nu/2} \quad (4.2)$$

and

$$z^2 = (1 - r^2/R^2), \quad (4.3)$$

as new dependent and independent variables, respectively.

Equation (4.1) is found to admit the general closed-form solution

$$\psi = A(1 - \tfrac{7}{2}z^2 + \tfrac{49}{24}z^4) + Bz(1 - \tfrac{7}{8}z^2)^{3/2}, \quad (4.4)$$

for the particular choice of geometric parameter $K = -7$, A and B being arbitrary constants of integration.

The space-time metric of this solution written out explicitly reads

$$ds^2 = -\frac{8-7z^2}{z^2}dr^2 - R^2(1-z^2)(d\theta^2 + \sin^2\theta\, d\phi)^2 + \left[A\left(1 - \frac{7}{2}z^2 + \frac{49}{24}z^4\right) + Bz\left(1 - \frac{7}{8}z^2\right)^{3/2}\right]^2 dt^2, \quad (4.5)$$

where $z^2 = 1 - r^2/R^2$.

The expressions for matter density and fluid pressure for the distribution of (4.5) are expressed as

$$\frac{8\pi G\rho}{c^2} = \frac{8}{R^2}\frac{10-7z^2}{(8-7z^2)^2} = \frac{24}{R^2}\frac{(1+\frac{7}{3}r^2/R^2)}{(1+7r^2/R^2)^2} \quad (4.6)$$

and

$$\frac{8\pi G p}{c^4} = \frac{A(-1+\frac{21}{4}z^2 - \frac{49}{12}z^4) - \frac{1}{4}Bz(5-7z^2)(1-\frac{7}{8}z^2)^{1/2}}{R^2(1-\frac{7}{8}z^2)\left[Bz(1-\frac{7}{8}z^2)^{3/2} + A(1-\frac{7}{2}z^2+\frac{49}{24}z^4)\right]}. \quad (4.7)$$

The solution (4.5) is a closed-form exact solution of Einstein's field equations representing a spherical fluid distribution at rest. Although it is not obtained on the basis of any explicit assumption about the interparticle interaction, it is a logical consequence of the potent geometrical structure assumed for the background space-time. Such closed-form solutions are expected to be of astrophysical interest provided they satisfy certain general basic requirements expected of the fluids at ultrahigh densities and pressures.

V. PHYSICAL REQUIREMENTS

In order that the solution (4.5) be physically meaningful one has to study carefully the implications of the following requirements it is expected to fulfill in its region of validity.

(i) The matter density ρ and fluid pressure p should be positive everywhere.

(ii) The gradients $d\rho/dr$ and dp/dr should be negative.

(iii) The speed of sound should be less than the speed of light.

(iv) The interior metric should be joined continuously with the exterior Schwarzschild metric,

$$ds^2 = -(1-2m/r)^{-1}dr^2 - r^2(d\theta^2 + \sin^2\theta\, d\phi^2) + (1-2m/r)dt^2, \quad (5.1)$$

as one crosses the boundary surface $r = a$ of the distribution. From the expression (4.6) if follows that $\rho > 0$ and further $d\rho/dr < 0$ throughout the distribution. Accordingly, the fluid sphere of the configuration is a regular fluid sphere in the sense introduced by Buchdahl.[3]

The equation for hydrostatic equilibrium in the form (3.10) implies that at all points $r < R$, if the pressure $p(r) > 0$, then the pressure gradient $dp/dr \leqslant 0$. At the center $r = 0$ of the distribution the density and pressure attain values ρ_0 and p_0 given by

$$8\pi G\rho_0/c^2 = 24/R^2, \quad (5.2)$$

$$\frac{8\pi G p_0}{c^4} = \frac{32}{R^2}\frac{(2\sqrt{2}A + 3B)}{(-22\sqrt{2}A + 3B)}, \quad (5.3)$$

respectively.

The pressure at the center p_0 will be positive if the arbitrary constants A and B comply with either

(a) $3B + 2\sqrt{2}A > 0$ and $3B - 22\sqrt{2}A > 0$

or

(b) $3B + 2\sqrt{2}A < 0$ and $3B - 22\sqrt{2}A < 0$.

We further impose the condition that $\rho - 3p/c^2 \geqslant 0$ the so-called strong energy conditions then at the center $\rho_0 - 3p_0/c^2 \geqslant 0$ and subsequently A and B should be further restricted to comply with

$$(10\sqrt{2}A + 3B)/(22\sqrt{2}A - 3B) \geqslant 0.$$

It is observed that A and B should be restricted so that either

$$A < 0, \quad -2\sqrt{2}A < 3B < -10\sqrt{2}A \quad (5.4)$$

or

$$A > 0, \quad -10\sqrt{2}A < 3B < -2\sqrt{2}A.$$

Equation (3.10) then implies that the pressure gradient will be negative in the central region and accordingly pressure

will be decreasing in the radially outward direction. We choose the surface $r = a$ where the pressure vanishes as the boundary surface of the distribution.

Across this boundary surface $r = a$, we join the interior metric (4.5) with the Schwarzschild exterior metric (5.1), stipulating the continuity of metric coefficients and also the continuity of pressure. Continuity of the metric coefficients give

$$\begin{aligned} m &= m(a) \\ &= \frac{4\pi G}{c^2}\int_0^a \xi^2 \rho(\xi)\, d\xi \\ &= \frac{4a^3}{R^2[1+7(a^2/R^2)]} \end{aligned} \tag{5.5}$$

and

$$\begin{aligned} (1-2m/a)^{1/2} = A(1-\tfrac{7}{2}z_a^2+\tfrac{49}{24}z_a^4) \\ + Bz_a(1-\tfrac{7}{8}z_a^2)^{3/2}, \end{aligned} \tag{5.6}$$

where $z_a^2 = 1 - a^2/R^2$.

The continuity of pressure across $r = a$ requires that pressure should vanish on the boundary implying that

$$\begin{aligned} A(-1+\tfrac{21}{4}z_a^2-\tfrac{49}{12}z_a^4) \\ = \tfrac{1}{4}Bz_a(1-\tfrac{7}{8}z_a^2)^{1/2}(5-7z_a^2). \end{aligned} \tag{5.7}$$

Conditions (5.6) and (5.7) determine the arbitrary constants A and B in terms of the curvature parameter R and the boundary radius a as

$$A = (5-7z_a^2)(1-2m/a)^{1/2}, \tag{5.8}$$

$$\begin{aligned} B = \frac{1}{z_a}\left(1-\frac{2m}{a}\right)^{1/2}\left(1-\frac{7}{8}z_a^2\right)^{-1/2} \\ \times\left(-4+21z_a^2-\frac{49}{3}z_a^4\right), \end{aligned} \tag{5.9}$$

where the total mass m is determined by (5.5).

VI. TOTAL MASS AND SIZE

The matter density, given by Eq. (4.6) attains the value ρ_a given by

$$\frac{8\pi G\rho_a}{c^2} = \frac{24}{R^2}\left(1+\frac{7}{3}\frac{a^2}{R^2}\right)\left(1+7\frac{a^2}{R^2}\right)^{-2}, \tag{6.1}$$

on the boundary $r = a$ of the distribution. Let

$$\lambda = \rho_a/\rho_0 \tag{6.2}$$

denote the ratio of the value of matter density on the boundary surface with its value at the center. Then evidently $\lambda < 1$ since ρ is a decreasing function of r, and represents a density-variation parameter, having the explicit expression

$$\lambda = \left(1+\frac{7}{3}\frac{a^2}{R^2}\right)\left(1+7\frac{a^2}{R^2}\right)^{-2}. \tag{6.3}$$

Equation (6.2) is a biquadratic equation in a/R that determines a/R in terms of λ as

$$a^2/R^2 = (1-6\lambda+\sqrt{(1+24\lambda)})/42\lambda, \tag{6.4}$$

the algebraic root assigning negative values to a^2/R^2 being rejected to ensure that a/R is real and positive.

Equation (5.2) determines geometric parameter R in terms of surface density ρ_a and density-variation parameter λ. Equation (6.4) determines the boundary radius "a" of the distribution and subsequently Eq. (5.5) determines the total mass of the configuration. Thus knowledge of the matter density on the boundary surface, ρ_a, and its ratio with the central density is enough to obtain estimates about the size and mass of the configuration.

In order to ensure that ρ and p be well behaved throughout the configuration we impose the restriction $dp/d\rho < c^2$, which implies that the speed of sound should not exceed speed of light c in the distribution.

A straightforward calculation using Eqs. (3.4) and (3.10) leads to

$$\begin{aligned} \frac{dp}{d\rho} = \frac{2\pi GR^2}{7}\frac{[1+7(r^2/R^2)]^3(\rho+p/c^2)}{(1-r^2/R^2)[5+7(r^2/R^2)]} \\ \times\left[1+\frac{\pi Gp}{c^4}\left(1+7\frac{r^2}{R^2}\right)R^2\right]. \end{aligned} \tag{6.5}$$

The values of $dp/d\rho$ range between its value at the center where the density is the highest and its value near the boundary surface where the density reaches its minimum value ρ_a.

At the center, $dp/d\rho$ has the value

$$\left(\frac{dp}{d\rho}\right)_0 = \frac{c^2R^2}{1120}\frac{8\pi G}{c^2}\left(\rho_0+\frac{p_0}{c^2}\right)\left(\frac{8\pi Gp_0R^2}{c^2}+8\right). \tag{6.6}$$

If we impose the condition $\rho_0 - 3p_0/c^2 > 0$ at the center then it readily follows that

$$\left(\frac{dp}{d\rho}\right)_0 < 0.46c^2 \tag{6.7}$$

on using the expression (5.2) for ρ_0.

At the boundary we have the expression

$$\left(\frac{dp}{d\rho}\right)_s = 2\pi GR^2\rho_a\left(1+7\frac{a^2}{R^2}\right)^3\Big/7\left(1-\frac{a^2}{R^2}\right)\left(5+7\frac{a^2}{R^2}\right) \tag{6.8}$$

for $dp/d\rho$ which can be expressed in the form

$$\left(\frac{dp}{d\rho}\right)_s = \frac{(1+\sqrt{(1+24\lambda)})^3}{(48\lambda-1-\sqrt{(1+24\lambda)})(1+24\lambda+\sqrt{(1+24\lambda)})}c^2 \tag{6.9}$$

using Eqs. (6.4) and (6.1). It is observed that for models with $0.2 \leqslant \lambda < 1$, $(dp/d\rho)_s < c^2$. In fact the requirement $dp/d\rho < c^2$ is observed to be satisfied throughout the distribution for models with $\lambda > 0.25$ and complying with the condition $\rho - p/c^2 \geqslant 0$, reported in Table I.

VII. SUPERDENSE STARS

A spherical star begins to contract under the influence of gravitational interaction of the matter content, when the thermonuclear sources of energy in its interior are exhausted. Its mass energy continues to increase and it ends up as a dense star—white dwarf, neutron star, or a black hole. The model proposed here describes a superdense star formed during these last stages of stellar evolution with densities in the range of $10^{14} \sim 10^{16}$ g cm^{-3}.

We take the matter density ρ_a on the boundary $r = a$ of the star as $\rho_a = 2 \times 10^{14}$ g cm^{-3}. Choosing different values for the density-variation parameter λ, for each value of λ, we determine the boundary radius a of the star and its total mass m, in accordance with the scheme of Sec. VI. The value of m obtained is in kilometers. The mass of the star in grams is obtained using $M = mc^2/G$. The results of these computations together with the values of the constants A and B as determined by the Eqs. (5.8) and (5.9) are given in Table I.

The first 13 values of λ in the table, i.e., $\lambda \geqslant 0.35$, give a set of physically viable models wherein equilibrium radius of each of these star-models is of the order of the radius of a neutron star. Both m and a are decreasing functions of λ. The maximum mass of the configuration is obtained at the equilibrium radius of 17.35 km for $\lambda = 0.35$. This maximum mass is closer to the limit on the maximum mass of neutron star imposed by the non-nuclear analysis of Rhodes and Ruffini. All these models comply with the conditions $\rho \geqslant 0$, $p \geqslant 0$, $\rho - 3p/c^2 \geqslant 0$, $d\rho/dr$, $dp/dr < 0$, $dp/d\rho < c^2$ throughout the configuration. However if we relax these conditions to $\rho - p/c^2 \geqslant 0$, complying with weak energy conditions, we can go as far as the first 15 values of λ in Table I; the model subsequently permitting higher values for m and a. One cannot go beyond that because in these models with $\lambda \leqslant 0.20$ the conditions $\rho - p/c^2 \geqslant 0$ and $dp/d\rho < c^2$ are not fulfilled within their configurations.

For the same values of the density-variation parameter the star models presented here have lesser values for equilibrium radius a and total mass m than the corresponding values for the star models obtained by Vaidya and Tikekar. The models presented here also permit more variation of density in the configuration without violating the physical requirements and admit the value for maximum mass that is close to the limiting value for maximum mass of a neutron star obtained by Rhodes and Ruffini.[9]

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Initial value formulation for the spherically symmetric dust solution

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An initial value formulation for the dust solution with spherical symmetry is given explicitly in which the initial distributions of dust and its velocity on an initial surface are chosen to be the initial data. As special cases, the Friedmann universe, the Schwarzschild solution in comoving coordinates, and a spherically symmetric and radially inhomogeneous cosmological model are derived.

I. INTRODUCTION

The general dust solution of spherical symmetry in comoving coordinates has been extensively studied[1-6] with the use of the metric[5]

$$ds^2 = dt^2 - Y'^2(t,r)/[1-\epsilon f^2(r)]dr^2 - Y^2(t,r)(d\theta^2 + \sin^2\theta\, d\varphi^2), \tag{1.1}$$

where $\epsilon = +1, -1, 0$; $Y'(t,r) = (\partial/\partial r)Y(t,r)$ and $f(r)$ is an arbitrary function of r. The Einstein field equation reads

$$\dot{Y}^2 - 2\mu(r)/Y = -\epsilon f^2(r), \tag{1.2}$$

where $\dot{Y} = (\partial/\partial t)Y(t,r)$ and $\mu(r)$ is another arbitrary function of r. The evolution of the mass density of the dust is

$$\rho(t,r) = \mu'/4\pi Y^2 Y'. \tag{1.3}$$

The solution of Eq. (1.2) can be expressed in a parametric form as

$$Y(t,r) = [\mu(r)/f^2(r)]h'(\eta), \tag{1.4}$$

$$h(\eta) = [f^3(r)/\mu(r)][t - n(r)], \tag{1.5}$$

where $n(r)$ is the third arbitrary function of r, $h'(\eta) = (d/d\eta)h(\eta)$, and $h(\eta)$ is defined by

$$h(\eta) = \begin{cases} \eta - \sin\eta, & \text{for } \epsilon = +1, \\ \frac{1}{6}\eta^3, & \text{for } \epsilon = 0, \\ \sinh\eta - \eta, & \text{for } \epsilon = -1. \end{cases} \tag{1.6}$$

Equations (1.1)–(1.6) constitute a complete set of exact solutions to the field equations for spherically symmetric dust in general relativity (with the cosmological constant $\Lambda = 0$). We see that there are three independent arbitrary functions $\mu(r)$, $f(r)$, and $n(r)$ to be determined for a given physical problem. Although one can, through a suitable specification for these three functions, produce a meaningful mass distribution $\rho(t,r)$, we do not know any general procedure by which the three functions can be determined explicitly for a reasonable physical system. The purpose of this paper is to look for such a procedure.

In Sec. II we treat the dust solution as an initial value problem. We find that by rescaling the radial coordinate, the number of independent arbitrary functions in the solution decreases by one to two. Instead of these two functions we choose another two functions, the initial distributions of the dust and its velocity, as initial data, and then we express the solution in an initial value formulation explicitly. In the following sections we use the general procedure given in Sec. II to discuss some simple examples: the Friedmann universe in Sec. III, the Schwarzschild solution in Sec. IV, and a spherically symmetric and radially inhomogeneous cosmological model in Sec. V.

II. INITIAL VALUE FORMULATION

We have noticed that the three arbitrary functions μ, f, and n depend on r solely and do not vary with time. This reminds us to treat the solution as an initial value problem.

As a first step we take the initial values of the complete set of field Eqs. (1.2) and (1.3) on an initial surface $t = t_i = \text{const}$, which give

$$\dot{Y}_i^2 - 2\mu/Y_i = -\epsilon f^2, \tag{2.1}$$

$$\rho_i = \mu'/4\pi Y_i^2 Y_i', \tag{2.2}$$

where

$$Y_i = Y_i(r) \equiv Y(t_i,r), \quad \dot{Y}_i = \dot{Y}_i(r) \equiv \dot{Y}(t_i,r),$$
$$\rho_i = \rho_i(r) \equiv \rho(t_i,r).$$

Here we get exactly three initial values: Y_i, $\dot{Y}_i$, and ρ_i. The first, Y_i, is the initial radial coordinate of comoving particles. The second and third, $\dot{Y}_i$ and ρ_i, are the initial velocity and the initial mass density, respectively. Here, $\dot{Y}_i$ and ρ_i are physical initial data while Y_i are coordinate initial data. Generally, Y_i is a function of r, therefore the indeterminacy in Y_i can be removed by rescaling the radial coordinate on the initial surface so as to make

$$Y_i(r) = ra_i, \tag{2.3}$$

where a_i is a constant. Let

$$Y(t,r) = ra(t,r), \tag{2.4}$$

then Eq. (2.3) implies $a(t_i,r) = a_i = \text{const}$.

Substituting Eq. (2.4) into Eq. (2.2) and integrating $\mu(r)$, we get

$$\mu(r) = 4\pi a_i^3 \int_0^r \rho_i r^2\, dr. \tag{2.5}$$

Substituting Eqs. (2.1) and (2.4) into Eq. (1.2), we get

$$\dot{a}^2 - 2\mu/ar^3 = \dot{a}_i^2 - 2\mu/a_i r^3. \tag{2.6}$$

This is the evolution equation of the scale factor $a(t,r)$. Equation (1.3) of the evolution of $\rho(t,r)$ can be written, through Eq. (2.5), as

$$\rho(t,r) = \rho_i a_i^3 a^{-2}/(ra)'. \tag{2.7}$$

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Equations (2.5), (2.6), and (2.7) constitute a complete set of field equations that can replace the original equations (1.2) and (1.3). For any given spherical dust system, the solution can be determined completely by this set of equations provided the initial data $\dot{a}_i$ and ρ_i are specified on the initial surface.

Now we should also express the solutions (1.4) and (1.5) in initial forms. Substituting Eq. (2.4) into Eq. (1.4) and taking its initial value, we obtain

$$f^2(r) = (\mu/a_i r)h'(\eta_i). \tag{2.8}$$

Then Eq. (1.4) is reduced to

$$a(t,r) = a_i[h'(\eta)/h'(\eta_i)]. \tag{2.9}$$

The arbitrary function $n(r)$ can be determined by taking the initial value of Eq. (1.5). Then substituting this $n(r)$ and Eq. (2.8) back into Eq. (1.5), we get

$$h(\eta) = h(\eta_i) \pm (1/\mu)[(\mu/a_i r)h'(\eta_i)]^{3/2}(t - t_i). \tag{2.10}$$

The initial value of the parameter η still needs to be determined. This can be achieved by differentiating Eqs. (2.9) and (2.10) with respect to t and then taking their initial values. The result can be written as

$$r^3 a_i \dot{a}_i^2/2\mu = [h''(\eta_i)]^2/2h'(\eta_i) = \begin{cases} \frac{1}{2}(1+\cos\eta_i), & \text{for } \epsilon = +1, \\ 1, & \text{for } \epsilon = 0, \\ \frac{1}{2}(1+\cosh\eta_i), & \text{for } \epsilon = -1. \end{cases} \tag{2.11}$$

We see that for the $\epsilon = 0$ case η_i is still undetermined. But in this case we in fact do not need to know the details of η_i. Directly from (2.10) we can obtain

$$\eta^3 = \eta_i^3[1 \pm (3/2a_i r)\sqrt{(2\mu/a_i r)}\,(t - t_i)], \quad \text{for } \epsilon = 0.$$

Therefore, from (2.9),

$$a = a_i[1 \pm (3/2a_i r)\sqrt{(2\mu/a_i r)}\,(t - t_i)]^{2/3}, \quad \text{for } \epsilon = 0. \tag{2.12}$$

The sign " $\pm$ " in Eqs. (2.10) and (2.12) should be chosen to meet the direction of the motion of the dust particles.

Thus the initial value formulation for the spherically symmetric dust solution are completed. We sum up the solution explicitly in the following equations:

$$ds^2 = dt^2 - a^2(t,r)\{[(1 + a^{-1}a')^2/(1 - kr^2)]dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\}, \tag{2.13}$$

$$k = 2\mu/a_i r^3 - \dot{a}_i^2, \quad \mu = 4\pi a_i^3 \int_0^r \rho_i r^2\, dr, \tag{2.14}$$

$$\dot{a}^2 + k = 2\mu/ar^3, \tag{2.15}$$

$$\rho = \rho_i a_i^3 a^{-2}/(ra)', \tag{2.16}$$

with a_i being a constant and $k, \mu, \dot{a}_i, \rho_i$ depend only on r. The solutions of Eq. (2.15) are as follows.

(i) $k > 0$:

$$a = a_i[(1 - \cos\eta)/(1 - \cos\eta_i)], \tag{2.17a}$$

$$\eta - \sin\eta = \eta_i - \sin\eta_i + (1/\mu)[(\mu/a_i r) \times (1 - \cos\eta_i)]^{3/2}(t - t_i), \tag{2.17b}$$

$$1 + \cos\eta_i = \mu^{-1} a_i \dot{a}_i^2 r^3. \tag{2.17c}$$

(ii) $k = 0$:

$$a = a_i[1 \pm (3/2a_i r)\sqrt{(2\mu/a_i r)}\,(t - t_i)]^{2/3}. \tag{2.18}$$

(iii) $k < 0$:

$$a = a_i[(\cosh\eta - 1)/(\cosh\eta_i - 1)], \tag{2.19a}$$

$$\sinh\eta - \eta = \sinh\eta_i - \eta_i \pm (1/\mu)[(\mu/a_i r) \times (\cosh\eta_i - 1)]^{3/2}(t - t_i), \tag{2.19b}$$

$$1 + \cosh\eta_i = \mu^{-1} a_i \dot{a}_i^2 r^3. \tag{2.19c}$$

Here the initial time t_i should be treated as a constant as usual.

Note that the initial quantities ρ_i and $\dot{a}_i$ can be any physically reasonable functions of r. So, generally, k and η_i are also functions of r. In the following sections we discuss some simple examples for ρ_i and $\dot{a}_i$.

III. FRIEDMANN UNIVERSE

Suppose

$$\rho_i = \text{const}, \quad \dot{a}_i = \text{const}, \tag{3.1}$$

then, from Eqs. (2.14),

$$\mu = \tfrac{4}{3}\pi\rho_i a_i^3 r^3, \quad k = \tfrac{8}{3}\pi\rho_i a_i^2 - \dot{a}_i^2, \tag{3.2}$$

so k is a constant. From Eqs. (2.17)–(2.19) we can show that η_i is also a constant and then a is independent of r. Thus Eqs. (2.15) and (2.16) reduce to

$$\dot{a}^2 + k = \tfrac{8}{3}\pi\rho_i a_i^3 a^{-1},$$

$$\rho = \rho_i a_i^3 a^{-3}, \tag{3.3}$$

and the line element (2.13) reduces to

$$ds^2 = dt^2 - a^2(t)[dr^2/(1 - kr^2) + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)]. \tag{3.4}$$

This is just the Friedmann universe.

IV. SCHWARZSCHILD SOLUTION

For Schwarzschild fields we can construct the comoving coordinates as follows. Imagine that the space is filled up with a dense cloud of freely falling test particles whose mass are negligible, and each particle is given a fixed radial coordinate label and carries along a little clock. The space-time coordinates r and t of any event are defined by taking r as the radial label of the particle that is just going by when and where the event occurs, and by taking t as the time then shown on that particle's clock. This coordinate system is useful throughout the region occupied by the particle cloud, for whatever interval of time in which particle trajectories do not cross.

In this comoving frame the initial distribution of the mass density should take the form

$$\rho_i(r) = m\delta^3(r), \tag{4.1}$$

where m is the total mass of the point source. Without loss of generality we set $a_i = 1$, then Eq. (2.14) gives

$$\mu = m. \tag{4.2}$$

By properly choosing the initial velocity $\dot{a}_i$, we obtain three

particular kinds of comoving coordinates for the Schwarzschild solution, which we list below without detailed calculation.

(i) $k>0$. We choose

$$\dot{a}_i = 0, \tag{4.3}$$

then $\eta_i = \pi$ and

$$\eta - \sin\eta = \pi + (2/r)\sqrt{2m/r}(t - t_i), \tag{4.4a}$$

$$ds^2 = dt^2 - \tfrac{1}{4}(1-\cos\eta)^2\{(1-2m/r)^{-1} \times\left[1 - \frac{3}{2}\frac{\sin\eta(\eta-\sin\eta-\pi)}{(1-\cos\eta)^2}\right]^2 dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\}. \tag{4.4b}$$

(ii) $k=0$.

$$ds^2 = dt^2 - \left[1 \pm (3/2r)\sqrt{2m/r}(t-t_i)\right]^{-2/3} dr^2 - \left[1 \pm (3/2r)\sqrt{2m/r}(t-t_i)\right]^{4/3} r^2(d\theta^2 + \sin^2\theta\, d\varphi^2). \tag{4.5}$$

(iii) $k<0$. We choose

$$\dot{a}_i^2 = 4m/r^3, \tag{4.6}$$

then

$$\cosh\eta_i = 3, \tag{4.7a}$$

$$\sinh\eta - \eta = \sinh\eta_i - \eta_i \pm (2/r)\sqrt{(2m/r)}\,(t - t_i), \tag{4.7b}$$

$$ds^2 = dt^2 - \tfrac{1}{4}(\cosh\eta - 1)^2\{(1+2m/r)^{-1} \times\left[1 - \frac{3}{2}\frac{\sinh\eta(\sinh\eta-\eta-\sinh\eta_i+\eta_i)}{(\cosh\eta-1)^2}\right]^2 dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\varphi^2)\}. \tag{4.7c}$$

We should point out that there are infinite kinds of comoving coordinates for the Schwarzschild solution, corresponding to different choices of the initial velocity $\dot{a}_i$. This just reflects a trivial fact that one can use test particles with different initial velocity to test the Schwarzschild fields. The work on the relation of these comoving coordinates to the standard Schwarzschild coordinates is in progress.

V. INHOMOGENEOUS COSMOLOGICAL MODELS

Generally, we can construct any spherically symmetric and radially inhomogeneous cosmological models. Here is a simple example.

Suppose

$$\rho_i(r) = \rho_c e^{-r/R}, \tag{5.1}$$

where ρ_c and R are two constants. Then, from Eqs. (2.14), we obtain

$$\mu(r) = 4\pi\rho_c a_i^3 R^3[2 - R^{-2}e^{-r/R}(r^2 + 2Rr + 2R^2)]. \tag{5.2}$$

From this equation we find

$$\lim_{r\to\infty}\mu(r) = 8\pi\rho_c a_i^3 R^3. \tag{5.3}$$

Thus we get a cosmological model in which the total matter of the universe is finite.

We can take an arbitrary choice for the initial velocity $\dot{a}_i$ of the dust in the model. For example, we choose

$$\dot{a}_i^2(r) = \alpha[2\mu(r)/a_i r^3], \quad \alpha = \text{const}, \tag{5.4}$$

then, from Eqs. (2.14), the three cases for $\alpha>1$, $\alpha=1$, and $\alpha<1$ correspond to $k<0$, $k=0$, and $k>0$, respectively. From Eqs. (2.17) and (2.19) we find that $\eta_i = \text{constant}$. The remaining calculation in Eqs. (2.13)–(2.19) are not very difficult.

VI. CONCLUSION

The general dust solution with spherical symmetry in comoving coordinates contains three arbitrary functions $\mu(r), f(r)$, and $n(r)$. It is of great significance to determine these functions for a given physical system. In this paper we have decreased the number of free functions from three to two by rescaling the radial coordinate on the initial surface. Then we have chosen two physically meaningful quantities, the initial mass density and the velocity of the dust, as initial data to reexpress the solution into an initial value formulation. Following this formulation we have derived, as special cases, the Friedmann universe, the Schwarzschild solution, and a spherically symmetric and radially inhomogeneous cosmological model containing finite matter. Some more applications in cosmology and astrophysics are also possible.

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Relativistic theory of spherically symmetric perturbation in dust universe

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Starting from the initial value formulation of dust solution given in the preceding paper [J. Math. Phys. **31**, 2459 (1990)] a relativistic perturbation equation and its general solutions in spherically symmetric universes are derived. It is found that these solutions are in analogy with the Bonnor–Weinberg results of the Newtonian theory and contain three modes: a growing mode, a decaying mode, and a constant mode.

I. INTRODUCTION

In the preceding paper[1] we have expressed the spherically symmetric dust solution of general relativity into an initial value formulation that can be summarized in the following.

The line element takes the form

$$ds^2 = dt^2 - a^2(t,r)\left[\frac{(1+a^{-1}a'r)^2}{1-kr^2}\,dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\gamma^2)\right], \tag{1.1}$$

with

$$k = 2\mu/a_i r^3 - \dot{a}_i^2, \tag{1.2a}$$

$$\mu = 4\pi a_i^3 \int_0^r \rho_i r^2\, dr, \tag{1.2b}$$

where prime and dot represent partial derivatives with respect to r and t, respectively; a_i, $\dot{a}_i$, and ρ_i are the initial values of the scale factor a, its expanding velocity $\dot{a}$, and the mass density ρ, respectively; and a_i is a constant and $\dot{a}_i, \rho_i, \mu$, and k depend only on r. The field equation is

$$\dot{a}^2 + k = 2\mu/ar^3, \tag{1.3}$$

and the evolution of the mass density is

$$\rho = \rho_i a_i^3 a^{-2}/(ra)'. \tag{1.4}$$

Suppose the universe is expanding at the initial time t_i, then the solutions of Eq. (1.3) are as follows.

(i) $k>0$:

$$a = a_i[(1-\cos\eta)/(1-\cos\eta_i)], \tag{1.5a}$$

$$\eta - \sin\eta = \eta_i - \sin\eta_i + (1/\mu)[(\mu/a_i r) \times (1-\cos\eta_i)]^{3/32}(t-t_i), \tag{1.5b}$$

$$1+\cos\eta_i = \mu^{-1} a_i \dot{a}_i^2 r^3. \tag{1.5c}$$

(ii) $k=0$:

$$a = a_i\left[1 + \frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}(t-t_i)\right]^{2/3}. \tag{1.6}$$

(iii) $k<0$:

$$a = a_i[(\cosh\eta - 1)/(\cosh\eta_i - 1)], \tag{1.7a}$$

$$\sinh\eta - \eta = \sinh\eta_i - \eta_i + (1/\mu)[(\mu/a_i r) \times (\cosh\eta_i - 1)]^{3/2}(t-t_i), \tag{1.7b}$$

$$1+\cosh\eta_i = \mu^{-1} a_i \dot{a}_i^2 r^3. \tag{1.7c}$$

Note that, generally, these solutions can describe any spherically symmetric cosmological models of dust universes. The isotropic and homogeneous Friedmann universe is just a particular model in which the initial velocity $\dot{a}_i$ and mass density ρ_i are constants.[1]

One of the most significant problems in cosmology is the formation of galaxies. The first Newtonian theory on this problem was proposed in 1902 by Jeans.[2] His theory uses a static fluid as the background and therefore does not describe the actual situation in our universe. The first relativistic theory of the instabilities in an expanding universe was given in 1946 by Lifshitz,[3] and an important development of Newtonian theory in describing an expanding universe was given in 1957 by Bonnor.[4] All of these works are well known, but we have noticed another useful way to think of the problem. That is, one can also use the spherical dust solution to study the spherical mode of the perturbation. It was shown[5] that the unperturbed Newtonian equations proposed by Zel'dovich[6] can be derived from the homogeneous Friedmann universe. A spherical perturbation will violate the radial homogeneity of the Friedmann universe but still has the spherical symmetry. Therefore, we expect that the spherical perturbation equations may be derived from the general dust solution. In fact, Lemaitre[7] was the first (of many) to notice that the dust solution is a pleasantly simple generalization of the usual homogeneous cosmological model. A detailed discussion for the spherical mode of the perturbation in dust universes was given by Peebles.[8] Now from Eqs. (1.1)–(1.7) we see that the dust solution has been successfully expressed into an initial value formulation with physically meaningful quantities ρ_i, the initial mass density, and $\dot{a}_i$, the initial expanding velocity of the universe, as initial data on the initial surface $t = t_i = \text{const}$. Therefore, we are now in a position to be able to treat the spherical mode of the perturbation as an initial value problem, and this is the purpose of this paper.

II. PERTURBATION EQUATION

There are three initial quantities a_i, $\dot{a}_i$, and ρ_i on the initial surface $t = t_i = \text{const}$, in which a_i is a constant and $\dot{a}_i$ and ρ_i are of physical significance. Now we seek the perturbation equations, by adding initial perturbations $\delta\dot{a}_i$ and $\delta\rho_i$ to the background quantities $\dot{a}_i$ and ρ_i on the initial surface. Since $\delta\dot{a}_i$ and $\delta\rho_i$ are also initial data, so they are functions of

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r only. Now insert $\delta\rho_i$ into Eq. (1.2b), we get a perturbation $\delta\mu$ as

$$\delta\mu = 4\pi a_i^3 \int_0^r \delta\rho_i\, r^2\, dr, \tag{2.1}$$

so $\delta\mu$ is also a function of r only. By using Eq. (1.2a) we rewrite the background equation (1.3) into the form

$$\dot{a}^2 - 2\mu/ar^3 = \dot{a}_i^2 - 2\mu/a_i r^3. \tag{2.2}$$

Then, to first-order in perturbations δa, $\delta\dot{a}$, $\delta\mu$, and $\delta\dot{a}_i$, this equation gives

$$\dot{a}\,\delta\dot{a} - \frac{\delta\mu}{ar^3} + \frac{\mu\,\delta a}{a^2 r^3} = \dot{a}_i\,\delta\dot{a}_i - \frac{\delta\mu}{a_i r^3}. \tag{2.3}$$

Since a_i keeps invariant in the perturbation, so δa must satisfy the constraint

$$\delta a(t = t_i, r) = \delta a_i = 0. \tag{2.4}$$

Without loss of generality we suppose

$$\delta a = (a/3\mu)\delta\mu + \delta a_1, \tag{2.5}$$

then by substituting this equation into Eq. (2.3) and using Eq. (2.2) again, we can reduce Eq. (2.3) into a simple form

$$\dot{a}\,\delta\dot{a}_1 + (\mu/a^2 r^3)\delta a_1 = A(r), \tag{2.6a}$$

where

$$A(r) = \dot{a}_i\,\delta\dot{a}_i - \left(\dot{a}_i^2 + \frac{\mu}{a_i r^3}\right)\frac{\delta\mu}{3\mu}. \tag{2.6b}$$

This is the fundamental differential equation that governs the growth or decay of the perturbations in expanding dust universes with spherical symmetry. The fractional change in density can be derived from Eq. (1.4) by keeping only the first order of perturbations,

$$\frac{\delta\rho}{\rho} = \frac{\delta\rho_i}{\rho_i} - \frac{2\delta a}{a} - \frac{(r\,\delta a)'}{(ra)'}. \tag{2.7}$$

Therefore, the density contrast $\delta\rho/\rho$ can be obtained from this equation if the solution of Eq. (2.6a) is known.

III. SOLUTIONS

There are two methods to obtain the perturbed solutions. The first is to integrate the perturbation equation (2.6a) directly. The second is to use the general solutions (1.5)–(1.7) because the perturbed field still has the spherical symmetry and still satisfies these equations.

A. Method (1): Integrating the perturbation equation (2.6a)

We find that the perturbation equation (2.6a) can be transformed into another form. Differentiating Eq. (2.2) with respect to t, we find

$$\mu/a^2 r^3 = -\ddot{a}. \tag{3.1}$$

Substituting this equation into Eq. (2.6a) we get

$$\dot{a}\,\delta\dot{a}_1 - \ddot{a}\,\delta a_1 = A(r), \tag{3.2}$$

then

$$\delta a_1 = A(r)\dot{a}\int \frac{dt}{\dot{a}^2}. \tag{3.3}$$

Combined with Eq. (2.5), we find

$$\frac{\delta a}{a} = \frac{\delta\mu}{3\mu} + A(r)\,\frac{\dot{a}}{a}\int \frac{dt}{\dot{a}^2}. \tag{3.4}$$

The scale factor $a(t,r)$ is given in Eqs. (1.5)–(1.7) for the three cases $k>0$, $k=0$, and $k<0$. Substituting these expressions of $a(t,r)$ into Eq. (3.4) and integrating it directly, we obtain the fractional change in scale factor $a(t,r)$ as follows.

(i) $k>0$:

$$\frac{\delta a}{a} = \frac{\delta\mu}{3\mu} + \frac{a_i r^3 A(r)}{\mu(1-\cos\eta_i)}\left[\frac{-3\eta\sin\eta}{(1-\cos\eta)^2} + \frac{5+\cos\eta}{1-\cos\eta} + C_1(r)\,\frac{\sin\eta}{(1-\cos\eta)^2}\right], \tag{3.5a}$$

$$C_1(r) = 3\eta_i - \frac{(5+\cos\eta_i)(1-\cos\eta_i)}{\sin\eta_i} - \frac{(1-\cos\eta_i)^3\delta\mu}{3a_i r^3 A(r)\sin\eta_i}. \tag{3.5b}$$

(ii) $k=0$:

$$\frac{\delta a}{a} = \frac{\delta\mu}{3\mu} + \frac{a_i r^3 A(r)}{5\mu}\left\{\left[1 + \frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}\,(t-t_i)\right]^{2/3} + C_2(r)\left[1 + \frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}\,(t-t_i)\right]^{-1}\right\}, \tag{3.6a}$$

$$C_2(r) = -1 - 5\delta\mu/3a_i r^3 A(r). \tag{3.6b}$$

(iii) $k<0$:

$$\frac{\delta a}{a} = \frac{\delta\mu}{3\mu} + \frac{a_i r^3 A(r)}{\mu(\cosh\eta_i - 1)}\left[\frac{-3\eta\sinh\eta}{(\cosh\eta-1)^2} + \frac{5+\cosh\eta}{\cosh\eta-1} + C_3(r)\,\frac{\sinh\eta}{(\cosh\eta-1)^2}\right], \tag{3.7a}$$

$$C_3(r) = 3\eta_i - \frac{(5+\cosh\eta_i)(\cosh\eta_i - 1)}{\sinh\eta_i} - \frac{(\cosh\eta_i - 1)^3\delta\mu}{3a_i r^3 A(r)\sinh\eta_i}. \tag{3.7b}$$

In the above equations, $C_1(r)$, $C_2(r)$, and $C_3(r)$ are constants of integration and are determined by Eq. (2.4), i.e., by the constraint that on the initial surface we must have $\delta a = 0$.

Compared to Eqs. (3.5)–(3.7) with the discussion given by Weinberg[9] we find that in all three cases of k, the fractional change in the scale factor $\delta a/a$ contains three modes: a growing mode $(\delta a/a)_+$, a decaying mode $(\delta a/a)_-$, and a constant mode $(\delta a/a)_0$. The constant mode is

$$\left(\frac{\delta a}{a}\right)_0 = \frac{\delta\mu}{3\mu}, \quad \text{for all } k, \tag{3.8}$$

and the other two modes are as follows.

(i) $k>0$:

$$\left(\frac{\delta a}{a}\right)_+ \propto \frac{-3\eta\sin\eta}{(1-\cos\eta)^2} + \frac{5+\cos\eta}{1-\cos\eta}, \tag{3.9a}$$

$$\left(\frac{\delta a}{a}\right)_- \propto C_1(r)\frac{\sin\eta}{(1-\cos\eta)^2}. \tag{3.9b}$$

(ii) $k=0$:

$$\left(\frac{\delta a}{a}\right)_+ \propto \left[1+\frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}(t-t_i)\right]^{2/3}, \tag{3.10a}$$

$$\left(\frac{\delta a}{a}\right)_- \propto C_2(r)\left[1+\frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}(t-t_i)\right]^{-1}. \tag{3.10b}$$

(iii) $k<0$:

$$\left(\frac{\delta a}{a}\right)_+ \propto \frac{-3\eta\sinh\eta}{(\cosh\eta-1)^2}+\frac{5+\cosh\eta}{\cosh\eta-1}, \tag{3.11a}$$

$$\left(\frac{\delta a}{a}\right)_- \propto C_3(r)\frac{\sinh\eta}{(\cosh\eta-1)^2}. \tag{3.11b}$$

We can see that all these expressions (3.9)–(3.11) are very analogous to those derived by Weinberg[9] based on the Newtonian theory with differences in two aspects. First, in Newtonian theory given by Bonnor[4] the growing mode and decaying mode are two independent solutions of the perturbation equation, while in the present theory the three modes are just different terms of a single solution of the equation and each has a definite coefficient. Second, in Newtonian theory the background field is the Friedmann universe, while in the present theory the background field can be any spherically symmetric dust universes that include the Friedmann universe as a special case.

B. Method (2): Using the general solutions (1.5)–(1.7)

Since the perturbed field still satisfies the general solutions (1.5)–(1.7), so we can seek the perturbed solutions by adding small perturbations $\delta\dot{a}_i$ and $\delta\mu$ directly to these solutions and keeping only the first-order perturbation terms. The results are listed in the following.

(i) $k>0$:

$$\delta a = a\left[\frac{\sin\eta}{1-\cos\eta}\delta\eta-\frac{\sin\eta_i}{1-\cos\eta_i}\delta\eta_i\right], \tag{3.12a}$$

$$\delta\eta=\frac{1-\cos\eta_i}{1-\cos\eta}\left\{\delta\eta_i+\left[\frac{3\sin\eta_i\,\delta\eta_i}{2(1-\cos\eta_i)}+\frac{\delta\mu}{2\mu}\right]\times\frac{\eta-\sin\eta-\eta_i+\sin\eta_i}{1-\cos\eta_i}\right\}, \tag{3.12b}$$

$$\delta\eta_i=-\frac{1+\cos\eta_i}{\sin\eta_i}\left(2\frac{\delta\dot{a}_i}{\dot{a}_i}-\frac{\delta\mu}{\mu}\right). \tag{3.12c}$$

(ii) $k=0$:

$$\frac{\delta a}{a}=\frac{\delta\mu}{3\mu}\left\{1-\left[1+\frac{3}{2a_i r}\sqrt{\frac{2\mu}{a_i r}}(t-t_i)\right]^{-1}\right\}. \tag{3.13}$$

(iii) $k<0$:

$$\delta a = a\left[\frac{\sinh\eta}{\cosh\eta-1}\delta\eta-\frac{\sinh\eta_i}{\cosh\eta_i-1}\delta\eta_i\right], \tag{3.14a}$$

$$\delta\eta=\frac{\cosh\eta_i-1}{\cosh\eta-1}\left\{\delta\eta_i+\left[\frac{3\sinh\eta_i\delta\eta_i}{2(\cosh\eta_i-1)}+\frac{\delta\mu}{2\mu}\right]\times\frac{\sinh\eta-\eta-\sinh\eta_i+\eta_i}{\cosh\eta_i-1}\right\}, \tag{3.14b}$$

$$\delta\eta_i=\frac{\cosh\eta_i+1}{\sinh\eta_i}\left(2\frac{\delta\dot{a}_i}{\dot{a}_i}-\frac{\delta\mu}{\mu}\right). \tag{3.14c}$$

After a straightforward and careful calculation with use of Eqs. (1.5), (1.7), and (2.6b), we obtain precisely the same results as Eqs. (3.5) and (3.7) for $k>0$ and $k<0$, respectively, with expressions $C_1(r)$ and $C_3(r)$ being determined automatically and without using the constraint (2.4). The result (3.13) of the $k=0$ case differs from Eqs. (3.6) by an absence of the growing mode. The reason is that the solution (1.6) requires precisely $\dot{a}_i^2=2\mu(a_i r^3)^{-1}$ (i.e., $k=0$), which gives $\dot{a}_i\delta\dot{a}_i=(a_i r^3)^{-1}\delta\mu$, and then $A(r)=0$, which reduce Eqs. (3.6) into (3.13). Generally, if the unperturbed universe is of $k=0$, then the perturbed universe must be of $k>0$ or $k<0$. Therefore, the general perturbed solution in $k=0$ case should be Eqs. (3.6).

IV. DISCUSSION

(i) The interpretation of the density perturbations in relativistic perturbation theory is a difficulty. While the density ρ is a scalar under coordinate transformations, the density perturbation $\delta\rho$ is not invariant under infinitesimal coordinate transformations; $\delta\rho$ is a gauge-dependent quantity.[10] Here, gauge is a choice of a one-to-one correspondence between points in the background space-time and points in the perturbed space-time. Different gauge choices can give different results for $\delta\rho$.[11] Therefore, we should clarify the meaning of the density perturbation $\delta\rho$ introduced in this paper. We know that the coordinate system in the dust solution (1.1)–(1.7) is a comoving proper-time orthogonal system in which t is the proper time of the dust particle and r is its radial coordinate label. Furthermore, the density perturbation introduced in Sec. II is of the definition

$$\delta\rho=\rho_p(t,r)-\rho_b(t,r), \tag{4.1}$$

where ρ_p is the density of the perturbed space-time and ρ_b is the density of the background space-time, both at the same proper time t and for dust particles having the same radial coordinate label r. Imagine that there are two $t=$ const comoving hypersurfaces; one is in the perturbed space-time and the other is in the background space-time. Then the constraint (2.4) tells us that at an initial moment these two hypersurfaces coincide and observers on these two hypersurfaces synchronize their clocks to read t_i and are assigned a same radial coordinate label r. It should be pointed out that at a followed moment these two hypersurfaces might be separated practically. Thus the density perturbation $\delta\rho$ introduced in this paper just measures the difference of the mass densities on these two hypersurfaces at the same proper time. The interpretation of other perturbation quantities, such as δa and $\delta\dot{a}$, is in analogy with $\delta\rho$. From the metric (1.1) and above discussion we can see that the gauge used in this paper also satisfies the synchronous gauge used in Refs. 8 and 9.

(ii) It is of great interest to compare the relativistic perturbation equation (2.6a) derived in Sec. II and the Newtonian perturbation equation derived by Bonnor. In order to do this we set $\delta a_1=a\epsilon$ in Eq. (2.6a), then differentiate it

with respect to t and use Eq. (3.1). Then we get

$$\ddot{\epsilon} + (2\dot{a}/a)\dot{\epsilon} - (3\mu/a^3r^3)\epsilon = 0. \tag{4.2}$$

If the background space-time is the isotropic and homogeneous Friedmann universe, we have[1]

$$\rho = \rho_i a_i{}^3 a^{-3}, \quad \mu = \tfrac{4}{3}\pi\rho a^3 r^3, \tag{4.3}$$

so Eq. (4.2) reduces to

$$\ddot{\epsilon} + (2\dot{a}/a)\dot{\epsilon} - 4\pi\rho\epsilon = 0. \tag{4.4}$$

This is just the Bonnor equation of perturbation based on the Newtonian theory with the pressure being ignored.[4,9]

(iii) Now we consider the $k = 0$ solution (1.6), from which we find that for particles with radial coordinate label r the beginning time t_s corresponds to $a(t_s,r) = 0$ and can be solved as

$$t_s = t_i - \frac{2a_i r}{3}\sqrt{\frac{a_i r}{2\mu(r)}}. \tag{4.5}$$

We see that generally t_s is not a constant but a function of r. Thus we arrive at a conclusion that particles in an inhomogeneous dust universe are not "created" at the same time as in the Friedmann universe. For the Friedmann universe we have

$$\mu = \tfrac{4}{3}\pi\rho_i a_i{}^3 r^3, \tag{4.6}$$

so, from (4.5), t_s is a constant for all particles in the universe. Therefore, we can reset the origin of the time axis so that $t = 0$ corresponds to the beginning time of the universe. Then Eq. (1.6) gives $a \propto t^{2/3}$, and, from (3.10) and (2.7), the perturbation modes in the $k = 0$ Friedmann universe are

$$\left(\frac{\delta\rho}{\rho}\right)_+ \propto \left(\frac{\delta a}{a}\right)_+ \propto t^{2/3}, \tag{4.7a}$$

$$\left(\frac{\delta\rho}{\rho}\right)_- \propto \left(\frac{\delta a}{a}\right)_- \propto t^{-1}, \tag{4.7b}$$

as are expected.

Finally, we should point out that if the perturbation quantities are not small compared to the corresponding background quantities, we still can use the general solutions (1.5)–(1.7) to determine the fractional changes of the scale factor $a(t,r)$ by, for instance, numerical method, and then to determine the density contrast $\delta\rho/\rho$ through Eq. (2.7).

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Stationarity of time correlation functions for globally linear classical systems and its consequences

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A necessary and sufficient condition for the stationarity of all time correlation functions associated with a given globally linear classical dynamical system is rigorously established from basic principles. Since stationarity of time correlation functions is a physical requirement that must be satisfied, the necessary and sufficient condition obtained for its realization represents a universal dynamical constraint on globally linear classical dynamical models intended to describe the execution of spontaneous fluctuations about a stationary state. This dynamical constraint is shown to (i) impose restrictions on the symmetry properties of the transition operator appearing in the global propagator for a system; (ii) represent a universal operator relation that embodies detailed balance and microscopic reversibility, giving rise to their traditional formulations; and (iii) imply the existence of certain generalized symmetry relations for time correlation functions and their Laplace and Fourier transforms. Apart from elucidating some fundamental symmetries of classical dynamical systems, the reported theory has the advantage of providing a simple model independent framework for treating classical time correlation functions via the extraction and utilization of dynamically embedded information. This is demonstrated in a concrete way by exploiting the mathematical apparatus of dual Lanczos transformation theory to determine the advanced and retarded components of the elements of the correlation matrices for first and second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator. The Laplace transforms of the retarded components of the time correlation functions and the Fourier transforms of the full-time correlation functions are also obtained.

I. INTRODUCTION

Recent work undertaken by us on the problem of determining spectral densities [Fourier transforms] of time correlation functions[1] via the extraction and utilization of dynamically embedded information[1,2] has prompted the following basic questions. (i) Do there exist constraints on the formal structure of the global propagator for a system? (ii) Do there exist symmetry constraints on the transition operator for a globally linear dynamical model intended to describe the execution of spontaneous fluctuations about a stationary state? The existence of such constraints is not only important from a fundamental point of view but is also important from the practical point of view in terms of the actual type of models that may be used to describe real physical systems.

In this paper, we establish that constraints on the global dynamics of classical systems do indeed exist. In particular, a necessary and sufficient condition for the stationarity[3,4] of all time correlation functions associated with a given globally linear classical dynamical system is rigorously established from basic principles. Since stationarity is a physical requirement that must be satisfied, the necessary and sufficient condition obtained by us for its realization represents a universal dynamical constraint on globally linear classical dynamical models intended to describe the execution of spontaneous fluctuations about a stationary state. We show that this dynamical constraint (i) imposes restrictions on the symmetry properties of the transition operator appearing in the global propagator for a system; (ii) represents a universal operator relation that embodies detailed balance and microscopic reversibility, giving rise to their traditional formulations;[3,5–7] and (iii) implies the existence of certain generalized symmetry relations for time correlation functions and their Laplace and Fourier transforms.

Apart from elucidating some fundamental symmetries of classical dynamical systems, the reported theory has the advantage of providing a simple model independent framework for treating classical time correlation functions via the extraction and utilization of dynamically embedded information.[1,2] This is demonstrated in a concrete way by exploiting the mathematical apparatus of dual Lanczos transformation theory[1,2,8] to determine the advanced and retarded components of the elements of the correlation matrices for first and second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.[1,8b,c,9] We also obtain the Laplace transforms[8c] of the retarded components

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of the time correlations functions and the Fourier transforms[1] of the full-time correlation functions.

II. BASIC STRUCTURE OF THE GLOBAL DYNAMICS

In order to determine the spectral density (Fourier transform) of a time correlation function, it is necessary to introduce a global propagator $\hat{U}(t)$ that bears information about the time-reversal properties of a system by including both the forward and backward time evolution.[1,10] The usual propagator $\exp(-\hat{L}t)$ is insufficient when the transition operator $\hat{L}$ possesses broken time-reversal symmetry, i.e., when $\tilde{L} \neq -\hat{L}$, where $\tilde{L}$ is the time-reversed form of $\hat{L}$. Of course, the usual propagator $\exp(-\hat{L}t)$ is sufficient when we are dealing with a reversible system, i.e., when the symmetry relation $\tilde{L} = -\hat{L}$ applies.

On the basis of time-reversal arguments, we can assert that the backward time evolution of a system is given by $\theta(-t)\exp(\tilde{L}t)$, where $\theta(-t)$ is the Heaviside step function. Hence, we write the global propagator $\hat{U}(t)$ in the form

$$\hat{U}(t) = \hat{U}^{>}(t) + \hat{U}^{<}(t), \tag{2.1}$$

where

$$\hat{U}^{>}(t) = \theta(t)\exp(-\hat{L}t) \tag{2.2}$$

and

$$\hat{U}^{<}(t) = \theta(-t)\exp(\tilde{L}t). \tag{2.3}$$

In the above, $\hat{U}^{>}(t)$ and $\hat{U}^{<}(t)$, respectively, describe the retarded (forward in time) and advanced (backward in time) dynamics of a system. The global propagator $\hat{U}(t)$ given by Eqs. (2.1)–(2.3) assumes the usual form $\hat{U}(t) = \exp(-\hat{L}t)$ for reversible systems when the substitution $\tilde{L} = -\hat{L}$ is made.

Note that $\hat{U}(t)$ possesses the following properties. (i) $\hat{U}(t) = \hat{U}^{>}(t)$ for $t>0$ and $\hat{U}(t) = \hat{U}^{<}(t)$ for $t<0$. (ii) $\lim_{t\to 0^+} \hat{U}(t) = \lim_{t\to 0^+} U^{>}(t) = 1$ and $\lim_{t\to 0^-} \hat{U}(t) = \lim_{t\to 0} \hat{U}^{<}(t) = 1$. (iii) $\hat{U}(t)$ is invariant with respect to the time-reversal transformation $\hat{L}, t \to \tilde{L}, -t$.

Property (iii) of the global propagator $\hat{U}(t)$ is common to both reversible and irreversible systems. Nonetheless, the transition operator $\hat{L}$, in general, possesses broken time-reversal symmetry even though the overall dynamics described by $\hat{U}(t)$ is time-reversal invariant.

The conditional transition probability $P(\Gamma',t\,|\Gamma,0)$ for the system of interest to pass from the phase point Γ to the phase point Γ' during the time interval t is given by

$$P(\Gamma',t\,|\Gamma,0) = U(\Gamma',\Gamma;t) \tag{2.4a}$$

$$= (\Gamma'|\hat{U}(t)|\Gamma), \tag{2.4b}$$

where $(\Gamma'|$ and $|\Gamma)$ are classical phase space state vectors (see Table I).

Introducing the global propagator $\hat{U}(t)$ into Eq. (2.4b), we resolve $P(\Gamma',t\,|\Gamma,0)$ into advanced and retarded components:

TABLE I. Properties of the classical phase space representation.

Definition of phase functions	$A(\Gamma) = (\Gamma\|A), A^*(\Gamma) = (\Gamma\|A^*)$
Orthonormality relation	$(\Gamma\|\Gamma') = \delta(\Gamma - \Gamma')$
Closure relation	$\hat{I} = \int d\Gamma\|\Gamma)(\Gamma\|$
Transition operator $\hat{L}$	$\hat{L} = \int d\Gamma \int d\Gamma'\|\Gamma)L(\Gamma,\Gamma')(\Gamma'\|$, where $L(\Gamma,\Gamma') = (\Gamma,\|\hat{L}\,|\Gamma'$. $L(\Gamma,\Gamma')$ is real by virtue of the requirement that $\rho(\Gamma;t)$ be real. So, $\hat{L}^\dagger = \hat{L}^T$.
Time-reversal transformation	$\hat{R} = \int d\Gamma \int d\Gamma\|\Gamma')R(\Gamma,\Gamma')(\Gamma'\|$, where $R(\Gamma,\Gamma') = \delta(\Gamma - \tilde{\Gamma}') = \delta(\tilde{\Gamma} - \Gamma')$.
operator $\hat{R}$	$R(\Gamma,\Gamma')$ is real. So, $\hat{R}^\dagger = \hat{R}^T$. $\hat{R}$ is a real orthogonal operator satisfying $\hat{R}^T\hat{R} = \hat{R}\hat{R}^T = \hat{I}, \hat{R}^T\hat{R}^T = \hat{R}\hat{R} = \hat{I}$, and $\hat{R}^T = \hat{R}$. Alternatively, $\hat{R}$ is a real unitary operator satisfying $\hat{R}^\dagger\hat{R} = \hat{R}\hat{R}^\dagger = \hat{I}, \hat{R}^\dagger\hat{R}^\dagger = \hat{R}\hat{R} = \hat{I}$, and $\hat{R}^\dagger = \hat{R}$.
Time-reversal transformations	$(\tilde{A}\,\| = (A\,\|\hat{R}$ and $\|\tilde{B}) = \hat{R}\,\|B)$, where $(\tilde{A}\,\|$ and $\|\tilde{B})$ are time-reversed dynamical vectors. $\hat{\tilde{L}} = \hat{R}\hat{L}\hat{R}$ is the time-reversed transition operator.
Nature of inner products $(A\,\|B)$ and $(A^*\|B)$	$(A\,\|B)$ is a symmetric inner product, i.e., $(A\,\|B) = (B\,\|A)$. $(A^*\|B)$ is a symmetric and Hermitian inner product, i.e., $(A^*\|B) = (B\,\|A^*)$ and $(A^*\|B) = (B^*\|A)^*$.
Relationship between vectors	$(A\,\| = \|A)^T, (\Gamma\| = \|\Gamma)^T$, and $\|\Gamma^*) = \|\Gamma)$. Also, $(A^*\| = \|A)^\dagger$ and $(\Gamma^*\| = \|\Gamma)^\dagger = \|\Gamma)^T$. The requirement that $(\Gamma^*\| = (\Gamma\|$ or $\|\Gamma^*) = \|\Gamma)$ follows from self-consistency arguments.
Conservation of probability	$(1\| = (1\|\exp(-\hat{L}t)$ for $t>0$ and $(1\| = (1\|\exp(\hat{\tilde{L}}t)$ for $t<0$, where $(1\| = \int d\Gamma(\Gamma\|$. Hence, $(0\| = (1\|\hat{L}^{l+1}$ and $(0\| = (1\|\hat{\tilde{L}}^{l+1}$ or $\int d\Gamma'\, L(\Gamma',\Gamma)^{(l+1)} = 0$ and $\int d\Gamma'\, L(\tilde{\Gamma}',\tilde{\Gamma})^{(l+1)} = 0$ for all $l\geq 0$ and accessible phase points $\{\Gamma\}$.
Detailed balance	$\tilde{L} = \hat{L}^T_{\rm EQ}$ or $L(\tilde{\Gamma},\tilde{\Gamma}') = L^T_{\rm EQ}(\Gamma,\Gamma')$

$$P(\Gamma',t\,|\Gamma,0) = P^{>}(\Gamma',t\,|\Gamma,0) + P^{<}(\Gamma',t\,|\Gamma,0), \quad (2.5)$$

where

$$P^{>}(\Gamma',t\,|\Gamma,0) = \hat{U}^{>}(\Gamma',\Gamma;t) \quad (2.6a)$$

$$= (\Gamma'|\hat{U}^{>}(t)|\Gamma) \quad (2.6b)$$

$$= \theta(t)(\Gamma'|\exp(-\hat{L}t)|\Gamma) \quad (2.6c)$$

and

$$P^{<}(\Gamma',t\,|\Gamma,0) = U^{<}(\Gamma',\Gamma;t) \quad (2.7a)$$

$$= (\Gamma'|\hat{U}^{<}(t)|\Gamma) \quad (2.7b)$$

$$= \theta(-t)(\Gamma'|\exp(\tilde{L}t)|\Gamma). \quad (2.7c)$$

It should be noted that $P(\Gamma',t\,|\Gamma,0) = P^{>}(\Gamma',t\,|\Gamma,0)$ for $t>0$ and $P(\Gamma',t\,|\Gamma,0) = P^{<}(\Gamma',t\,|\Gamma,0)$ for $t<0$. Also, note that $P(\Gamma',t\,|\Gamma,0)$, $P^{>}(\Gamma',t\,|\Gamma,0)$, and $P^{<}(\Gamma',t\,|\Gamma,0)$ satisfy the initial conditions

$$\lim_{t\to 0^+} P(\Gamma',t\,|\Gamma,0) = \lim_{t\to 0^+} P^{>}(\Gamma',t\,|\Gamma,0) \quad (2.8a)$$

$$= \delta(\Gamma'-\Gamma) \quad (2.8b)$$

and

$$\lim_{t\to 0^-} P(\Gamma',t\,|\Gamma,0) = \lim_{t\to 0^-} P^{<}(\Gamma',t\,|\Gamma,0) \quad (2.9a)$$

$$= \delta(\Gamma'-\Gamma) \quad (2.9b)$$

by virtue of the orthonormality relation $(\Gamma'|\Gamma) = \delta(\Gamma'-\Gamma)$ (see Table I).

Assuming that we are working with a closed system, $P(\Gamma',t\,|\Gamma,0)$, $P^{>}(\Gamma',t\,|\Gamma,0)$, and $P^{<}(\Gamma',t\,|\Gamma,0)$ are properly normalized, i.e.,

$$\int_{\mathcal{Q}} d\Gamma'\, P(\Gamma',t\,|\Gamma,0) = 1$$

for all t, (2.10)

$$\int_{\mathcal{Q}} d\Gamma'\, P^{>}(\Gamma',t\,|\Gamma,0) = 1$$

for $t>0$, (2.11)

and

$$\int_{\mathcal{Q}} d\Gamma'\, P^{<}(\Gamma',t\,|\Gamma,0) = 1$$

for $t<0$, (2.12)

where the integration over Γ' is restricted to the accessible phase space $\mathcal{Q}$. The above may be readily established from the conservation of probability relations

$$\int_{\mathcal{Q}} d\Gamma(\Gamma|\exp(-\hat{L}t) = \int_{\mathcal{Q}} d\Gamma(\Gamma|$$

for $t>0$ and

$$\int_{\mathcal{Q}} d\Gamma(\Gamma|\exp(\tilde{L}t) = \int_{\mathcal{Q}} d\Gamma(\Gamma|$$

for $t<0$ (see Table I).

It follows from Eqs. (2.6c) and (2.7c) [also, see Table I.] that the retarded and advanced components of the conditional transition probability $P(\Gamma',t\,|\Gamma,0)$ satisfy the symmetry relations

$$P^{>}(\Gamma',t\,|\Gamma,0) = P^{<}(\tilde{\Gamma}',-t\,|\tilde{\Gamma},0) \quad (2.13)$$

and

$$P^{<}(\Gamma',t\,|\Gamma,0) = P^{>}(\tilde{\Gamma}',-t\,|\tilde{\Gamma},0), \quad (2.14)$$

where $\tilde{\Gamma} = (-\mathbf{p},\mathbf{q})$ is the time-reversed phase point corresponding to the phase point $\Gamma = (\mathbf{p},\mathbf{q})$, with $\mathbf{p}$ and $\mathbf{q}$, respectively, denoting the collective momentum and collective coordinate vectors for the particles of interest.

Making use of Eqs. (2.5), (2.13), and (2.14), we find that the conditional transition probability $P(\Gamma',t\,|\Gamma,0)$ possesses the symmetry

$$P(\Gamma',t\,|\Gamma,0) = P(\tilde{\Gamma}',-t\,|\tilde{\Gamma},0). \quad (2.15)$$

It should be noted that this symmetry relation and those given by Eqs. (2.13) and (2.14) apply independent of whether or not the transition operator $\hat{L}$ possesses broken time-reversal symmetry. The symmetry property given by Eq. (2.15) is usually associated only with globally reversible systems.[11]

III. NECESSARY AND SUFFICIENT CONDITION FOR STATIONARITY

Consider the equilibrium averaged time correlation function $C_{A,B}(t)$ characterizing the correlation between the classical dynamical variables $A(\Gamma)$ and $B(\Gamma)$ for a closed classical system for all time t, including $t<0$ and $t>0$. We define $C_{A,B}(t)$ by[3]

$$C_{A,B}(t) = \langle\langle A(t)B(0)\rangle\rangle_{\mathrm{EQ}} \quad (3.1a)$$

$$= \int_{\mathcal{Q}} d\Gamma \int_{\mathcal{Q}} d\Gamma'\, A(\Gamma')P(\Gamma',t\,|\Gamma,0) \times B(\Gamma)\rho_{\mathrm{EQ}}(\Gamma), \quad (3.1b)$$

where $\rho_{\mathrm{EQ}}(\Gamma)$ is the equilibrium probability density at the phase point Γ. The double bracket notation in Eq. (3.1a) has been used to indicate that the time correlation function $\ll A(t)B(0)\gg_{\mathrm{EQ}}$ describes fluctuations in both the forward and backward directions of time.

With the resolution given by Eq. (2.5), we can resolve the time correlation function $C_{A,B}(t)$ into retarded and advanced components:

$$C_{A,B}(t) = C^{>}_{A,B}(t) + C^{<}_{A,B}(t), \quad (3.2)$$

where

$$C^{>}_{A,B}(t) = \int_{\mathcal{Q}} d\Gamma \int_{\mathcal{Q}} d\Gamma'\, A(\Gamma')P^{>}(\Gamma',t\,|\Gamma,0) \times B(\Gamma)\rho_{\mathrm{EQ}}(\Gamma) \quad (3.3)$$

and

$$C^{<}_{A,B}(t) = \int_{\mathcal{Q}} d\Gamma \int_{\mathcal{Q}} A(\Gamma')P^{<}(\Gamma',t\,|\Gamma,0) \times B(\Gamma)\rho_{\mathrm{EQ}}(\Gamma). \quad (3.4)$$

Making use of the inner products $(A\,|\Gamma') = A(\Gamma')$ and $(\Gamma|B\rho_{\mathrm{EQ}}) = B(\Gamma)\rho_{\mathrm{EQ}}(\Gamma)$ and the closure relation $\hat{I} = \int_{\mathcal{Q}} d\Gamma|\Gamma)(\Gamma|$ (see Table I), we cast $C_{A,B}(t)$, $C^{>}_{A,B}(t)$, and $C^{<}_{A,B}(t)$ into the following forms:

$$C_{A,B}(t) = (A|\hat{U}(t)|B\rho_{EQ}) \tag{3.5a}$$

$$= \theta(t)(A|\exp(-\hat{L}t)|B\rho_{EQ}) + \theta(-t)(A|\exp(\tilde{L}t)|B\rho_{EQ}), \tag{3.5b}$$

$$C^{>}_{A,B}(t) = (A|\hat{U}^{>}(t)|B\rho_{EQ}) \tag{3.6a}$$

$$= \theta(t)(A|\exp(-\hat{L}t)|B\rho_{EQ}), \tag{3.6b}$$

and

$$C^{<}_{A,B}(t) = (A|\hat{U}^{<}(t)|B\rho_{EQ}) \tag{3.7a}$$

$$= \theta(-t)(A|\exp(\tilde{L}t)|B\rho_{EQ}). \tag{3.7b}$$

Let us make use of Eq. (3.5b) to establish that the symmetry relation

$$\tilde{L} = \hat{L}^{T}_{EQ} \tag{3.8}$$

is a necessary and sufficient condition for the time correlation function $C_{A,B}(t)$ to be stationary, as embodied in the relation[3,4]

$$C_{A,B}(t) = C_{B,A}(-t) \tag{3.9}$$

or

$$\langle\langle A(t)B(0)\rangle\rangle_{EQ} = \langle\langle B(-t)A(0)\rangle\rangle_{EQ}, \tag{3.10}$$

for all dynamical variables A and B.

The operator $\hat{L}^{T}_{EQ}$ appearing in Eq. (3.8) is the transpose of the transformed transition operator

$$\hat{L}_{EQ} = \hat{S}^{-1}_{EQ}\hat{L}\hat{S}_{EQ}, \tag{3.11}$$

where the operators $\hat{S}_{EQ}$ and $\hat{S}^{-1}_{EQ}$ are defined in such a way that $\hat{S}_{EQ}|A) = |A\rho_{EQ})$, $\hat{S}^{-1}_{EQ}|A\rho_{EQ}) = |A)$, $(A|\hat{S}_{EQ} = (A\rho_{EQ}|$, and $(A\rho_{EQ}|\hat{S}^{-1}_{EQ} = (A|$. Also, $\hat{S}_{EQ}$ and $\hat{S}^{-1}_{EQ}$ possess the properties $\hat{S}_{EQ}\hat{S}^{-1}_{EQ} = \hat{S}^{-1}_{EQ}\hat{S}_{EQ} = \hat{I}$, $\hat{S}^{T}_{EQ} = \hat{S}_{EQ}$, and $(\hat{S}^{-1}_{EQ})^{T} = \hat{S}^{-1}_{EQ}$.

Making use of the transformation given by Eq. (3.11) and the properties of the operators $\hat{S}_{EQ}$ and $\hat{S}^{-1}_{EQ}$, we write Eq. (3.5b) in the form

$$C_{A,B}(t) = \theta(t)(A\rho_{EQ}|\exp(-\hat{L}_{EQ}t)|B) + \theta(-t)(A\rho_{EQ}|\exp(\tilde{L}_{EQ}t)|B). \tag{3.12}$$

This equation may be rewritten as

$$C_{A,B}(t) = \theta(t)(B|\exp(-\hat{L}^{T}_{EQ}t)|A\rho_{EQ}) + \theta(-t)(B|\exp(\tilde{L}^{T}_{EQ}t)|A\rho_{EQ}). \tag{3.13}$$

It is clear from Eq. (3.5b) that

$$C_{B,A}(-t) = \theta(t)(B|\exp(-\tilde{L}t)|A\rho_{EQ}) + \theta(-t)(B|\exp(\hat{L}t)|A\rho_{EQ}). \tag{3.14}$$

Upon comparing this equation with Eq. (3.13), we conclude that the symmetry relation given by Eq. (3.8) is a necessary and sufficient condition for the time correlation function $C_{A,B}(t)$ to be stationary, as embodied in Eq. (3.9), for all dynamical variables A and B.

Since the stationarity condition given by Eq. (3.9) or (3.10) is a physical requirement that must be satisfied, it is clear that the necessary and sufficient condition given by Eq. (3.8) for its realization represents a universal dynamical constraint on globally linear classical dynamical models intended to describe the execution of spontaneous fluctuations about a stationary state. If this constraint is not satisfied, stationarity will be violated for some or perhaps all dynamical variables.

Since the transition operator $\hat{L}$ must conform to Eq. (3.8), Eq. (3.5b) may be cast into the form

$$C_{A,B}(t) = \theta(t)(A|\exp(-\hat{L}t)|B\rho_{EQ}) + \theta(-t)(B|\exp(\hat{L}t)|A\rho_{EQ}). \tag{3.15}$$

In writing Eq. (3.15), we have made use of the fact that the advanced component $C^{<}_{A,B}(t)$ [see Eqs. (3.2), (3.5b), and (3.7b)] of $C_{A,B}(t)$ may be written

$$C^{<}_{A,B}(t) = \theta(-t)(B|\exp(\hat{L}t)|A\rho_{EQ}) \tag{3.16}$$

by virtue of Eq. (3.8).

Note that the universal dynamical constraint given by Eq. (3.8) has allowed us to write both the retarded and advanced components of the time correlation function $C_{A,B}(t)$ in terms of matrix elements of the usual propagator $\exp(-\hat{L}t)$. Apart from the Heaviside step function, the matrix element $(A|\exp(-\hat{L}t)|B\rho_{EQ})$ is simply the equilibrium-averaged time correlation function $\langle A(t)B(0)\rangle_{EQ}$ characterizing the correlation between the dynamical variables A and B in the forward direction of time. Making use of this identification, we write $C_{A,B}(t)$, $C^{>}_{A,B}(t)$, and $C^{<}_{A,B}(t)$ in the more transparent forms

$$C_{A,B}(t) = \theta(t)\langle A(t)B(0)\rangle_{EQ} + \theta(-t)\langle\tilde{A}(-t)\tilde{B}(0)\rangle_{EQ} \tag{3.17a}$$

$$= \theta(t)\langle A(t)B(0)\rangle_{EQ} + \theta(-t)\langle B(-t)A(0)\rangle_{EQ}, \tag{3.17b}$$

$$C^{>}_{A,B}(t) = \theta(t)\langle A(t)B(0)\rangle_{EQ}, \tag{3.18}$$

and

$$C^{<}_{A,B}(t) = \theta(-t)\langle\tilde{A}(-t)\tilde{B}(0)\rangle_{EQ} \tag{3.19a}$$

$$= \theta(-t)\langle B(-t)A(0)\rangle_{EQ}. \tag{3.19b}$$

The tilde in Eqs. (3.17a) and (3.19a) indicates that $\tilde{A}$ and $\tilde{B}$ are time-reversed dynamical variables, i.e., $\tilde{A}(\Gamma) = A(\tilde{\Gamma})$ and $\tilde{B}(\Gamma) = B(\tilde{\Gamma})$.

One can easily see from Eqs. (3.15) and (3.17b) that the time correlation function $C_{A,B}(t)$ does indeed conform to the stationarity condition given by Eq. (3.9). Nonetheless, the time correlation functions $\langle A(t)B(0)\rangle_{EQ}$, $\langle\tilde{A}(-t)\tilde{B}(0)\rangle_{EQ}$, and $\langle B(-t)A(0)\rangle_{EQ}$ appearing in Eqs. (3.17a)–(3.19b) are not stationary unless the symmetry relations $\hat{L}_{EQ} = \hat{L}$ [see Eq. (3.8)] and $\tilde{\hat{L}} = -\hat{L}$ apply, i.e., the underlying dynamics is reversible. In fact, one can easily use our operator language to establish that the symmetry relations $\hat{L}_{EQ} = \hat{L}$ and $\tilde{\hat{L}} = -\hat{L}$ represent a necessary and sufficient condition for the time correlation function $\langle A(t)B(0)\rangle_{EQ}$ to be stationary for all dynamical variables A and B. For such cases, we have

$$C_{A,B}(t) = \langle A(t)B(0)\rangle_{EQ} \tag{3.20a}$$

$$= \langle B(-t)A(0)\rangle_{EQ}. \tag{3.20b}$$

IV. CONSEQUENCES OF THE UNIVERSAL DYNAMICAL CONSTRAINT

Now that we have established that Eq. (3.8) is a universal dynamical constraint on globally linear classical dynamical models, let us proceed to explore its consequences.

A. Stationary property of the equilibrium probability density

It is obvious from the properties of $\hat{S}_{\rm EQ}$ and $\hat{S}_{\rm EQ}^{-1}$ that $(0|\hat{S}_{\rm EQ} = (0|$ and $(1|\hat{S}_{\rm EQ} = (\rho_{\rm EQ}|$. Making use of these relations, the conservation of probability relation $(1|\hat{\tilde{L}} = (0|$ (see Table I), and the dynamical constraint given by Eq. (3.8), we find that $(\rho_{\rm EQ}|\hat{L}^T = (0|$ or $\hat{L}\,|\rho_{\rm EQ}) = |0)$. Hence, the state vector $|\rho_{\rm EQ})$ is stationary with respect to the retarded dynamics [see Eq. (2.2)].

Now making use of the identity $\hat{L}\,|\tilde{\rho}_{\rm EQ}) = \hat{R}\hat{\tilde{L}}\,|\rho_{\rm EQ})$ [see Table I], the conservation of probability relation $\hat{L}^T|1) = |0)$, see Table I, and the dynamical constraint given by Eq. (3.8), we obtain $\hat{\tilde{L}}\,|\tilde{\rho}_{\rm EQ}) = |0)$ or $\hat{\tilde{L}}\,|\rho_{\rm EQ}) = |0)$. Hence, the state vector $|\rho_{\rm EQ})$ is stationary with respect to the advanced dynamics [see Eq. (2.3)]. Combining this result with the result of the preceeding paragraph, we conclude that the universal dynamical constraint given by Eq. (3.8) and the conservation of probability ensure that $|\rho_{\rm EQ})$ is stationary with respect to the global dynamics, i.e., $\hat{U}(t)|\rho_{\rm EQ}) = |\rho_{\rm EQ})$ [see Eqs. (2.1)–(2.3)].

B. Detailed balance and microscopic reversibility

The dynamical constraint given by Eq. (3.8) assumes the following form in the classical phase space representation (see Table I):

$$L(\tilde{\Gamma},\tilde{\Gamma}') = L^{T}_{\rm EQ}(\Gamma,\Gamma'), \tag{4.1}$$

where

$$L_{\rm EQ}(\Gamma,\Gamma') = \rho^{-1}_{\rm EQ}(\Gamma)L(\Gamma,\Gamma')\,\rho_{\rm EQ}(\Gamma'). \tag{4.2}$$

Introducing Eq. (4.2) into Eq. (4.1), we obtain the following version of the principle of detailed balance for the matrix elements $\{L(\Gamma,\Gamma')\}$ of the transition operator $\hat{L}$:

$$L(\Gamma,\Gamma')\rho_{EQ}(\Gamma') = L(\tilde{\Gamma}',\tilde{\Gamma})\rho_{\rm EQ}(\tilde{\Gamma}), \tag{4.3a}$$

$$= \rho_{\rm EQ}(\tilde{\Gamma})L^{T}(\tilde{\Gamma},\tilde{\Gamma}'), \tag{4.3b}$$

where the equality $\rho_{\rm EQ}(\tilde{\Gamma}) = \rho_{\rm EQ}(\Gamma)$ is assumed.

Examples of globally linear classical dynamical models conforming to Eqs. (4.3a) and (4.3b) are displayed in Table II for the case of 1-D systems. In defining the transpose $L^{T}(\Gamma,\Gamma')$ in Table II, we have made use of the relation

$$\int_{\mathcal{D}} d\Gamma \int_{\mathcal{D}} d\Gamma'\, \psi(\Gamma)L(\Gamma,\Gamma')\chi(\Gamma') = \int_{\mathcal{D}} d\Gamma \int_{\mathcal{D}} d\Gamma'\, \chi(\Gamma)L^{T}(\Gamma,\Gamma')\psi(\Gamma') \tag{4.4}$$

and assumed that the phase functions $\psi(\Gamma)$ and $\chi(\Gamma)$ are of such a character that the surface contributions may be neglected. This assumption is equivalent to asserting that we are dealing with a closed classical dynamical system and that the phase functions $\psi(\Gamma)$ and $\chi(\Gamma)$ satisfy the appropriate boundary conditions for ensuring the conservation of probability.[12]

In writing Eqs. (4.3a) and (4.3b), we have allowed for the use of both local and nonlocal dynamical models in the

TABLE II. Matrix elements of the dimensionless operators $\hat{\tilde{L}}$, $\hat{\tilde{L}}_{\rm EQ}$, and $\hat{\tilde{L}}^{T}$ in the classical phase space representation for "single particle, 1-D classical systems" described by Liouville, Fokker–Planck, Smoluchowski, and BGK dynamics.

Dynamics	Matrix elements of $\overline{L}$, $\overline{L}_{\rm EQ}$, and $\overline{L}^{T}$[a,b,c,d]
Liouville	$\overline{L}(\bar{p},\bar{q};\bar{p}',\bar{q}') = [\bar{p}(\partial/\partial\bar{q}) + \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{p}-\bar{p}')\delta(\bar{q}-\bar{q}')$ $\overline{L}_{\rm EQ}(\bar{p},\bar{q};\bar{p}',\bar{q}') = [\bar{p}(\partial/\partial\bar{q}) + \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{p}-\bar{p}')\delta(\bar{q}-\bar{q}')$ $\overline{L}^{T}(\bar{p},\bar{q};\bar{p}',\bar{q}') = [-\bar{p}(\partial/\partial\bar{q}) - \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{q}-\bar{q}')$
Fokker–Planck	$\overline{L}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[\bar{p}(\partial/\partial\bar{q}) + \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})] - \eta(\partial/\partial\bar{p})[\bar{p} + (\partial/\partial\bar{p})]\}\delta(\bar{p}-\bar{p}')\delta(\bar{q}-\bar{q}')$ $\overline{L}_{\rm EQ}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[\bar{p}(\partial/\partial\bar{q}) + \epsilon F(\bar{q})(\partial/\partial\bar{p})] + \eta[\bar{p}(\partial/\partial\bar{p}) - (\partial^2/\partial\bar{p}^2)]\}\delta(\bar{p}-\bar{p}')\delta(\bar{q}-\bar{q}')$ $\overline{L}^{T}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[-\bar{p}(\partial/\partial\bar{q}) - \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})] + \eta[\bar{p}(\partial/\partial\bar{p}) - (\partial^2/\partial\bar{p}^2)]\}\delta(\bar{p}-\bar{p}')\delta(\bar{q}-\bar{q}')$
BGK	$\overline{L}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[\bar{p}(\partial/\partial\bar{q}) + \epsilon F(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{p}-\bar{p}') - g[\bar{p}_{\bar{p},\rm EQ}(\bar{p}) - \delta(\bar{p}-\bar{p}')]\}\delta(\bar{q}-\bar{q}')$ $\overline{L}_{\rm EQ}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[-\bar{p}(\partial/\partial\bar{q}) - \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{p}-\bar{p}') - g[\bar{p}_{\bar{p},\rm EQ}(\bar{p}') - \delta(\bar{p}-\bar{p}')]\}\delta(\bar{q}-\bar{q}')$ $\overline{L}^{T}(\bar{p},\bar{q};\bar{p}',\bar{q}') = \{[-\bar{p}(\partial/\partial\bar{q}) - \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{p})]\delta(\bar{p}-\bar{p}') - g[\bar{p}_{\bar{p},\rm EQ}(\bar{p}') - \delta(\bar{p}-\bar{p}')]\}\delta(\bar{q}-\bar{q}')$
Smoluchowski	$\overline{L}(\bar{q};\bar{q}') = -(1/\eta)(\partial/\partial\bar{q})[(\partial/\partial\bar{q}) - \epsilon\overline{F}(\bar{q})]\delta(\bar{q}-\bar{q}')$ $\overline{L}_{\rm EQ}(\bar{q};\bar{q}') = -(1/\eta)[(\partial^2/\partial\bar{q}^2) + \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{q})]\delta(\bar{q}-\bar{q}')$ $\overline{L}^{T}(\bar{q};\bar{q}') = -(1/\eta)[(\partial^2/\partial\bar{q}^2) + \epsilon\overline{F}(\bar{q})(\partial/\partial\bar{q})]\delta(\bar{q}-\bar{q}')$

[a] $\epsilon = (\epsilon_S/k_{\rm B}T)$, where ϵ_S is the energy scale, $k_{\rm B}$ is Boltzmann's constant, and T is the equilibrium temperature. $\eta = (m\beta_f^2 q_S^2/k_{\rm B}T)^{1/2} = (q_S^2 k_{\rm B}T/mD^2)^{1/2}$ and $g = (mf_c^2 q_S^2/k_{\rm B}T)^{1/2}$, where β_f is the friction coefficient in Fokker–Planck dynamics, D is the diffusion coefficient in Smoluchowski dynamics, f_c is the collisional frequency in BGK dynamics, m is the mass of the particle of interest, and q_S is the length scale. $\bar{q}$ is the dimensionless coordinate $\bar{q} = q/q_S$ and $\bar{p}$ is the dimensionless momentum $\bar{p} = p/p_S$, where $p_S = (mk_{\rm B}T)^{1/2}$. The dimensionless force $\overline{F}(\bar{q}) = -(d/d\bar{q})\overline{U}(\bar{q})$ has been introduced by writing $U(q) = \epsilon_S\overline{U}(\bar{q})$. $\hat{\tilde{L}} = t_S\hat{L}$, where $t_S = (mq_S^2/k_{\rm B}T)^{1/2}$ is the time scale.

[b] $\bar{p}$ and $\bar{p}'$ in the symbol $\overline{L}(\bar{p},\bar{q};\bar{p}',\bar{q}')$ is suppressed for the case of Smoluchowski dynamics.

[c] $\overline{L}_{\rm EQ}(\bar{p},\bar{q};\bar{p}',\bar{q}')$ has been determined by using the dimensionless canonical equilibrium probability density $\overline{\rho}_{\rm EQ}(\bar{p},\bar{q}) = Z^{-1}\exp[-(\frac{1}{2})\bar{p}^2 - \epsilon\overline{U}(\bar{q})]$, where $\overline{Z} = \int d\bar{p}\int d\bar{q}\exp[-(\frac{1}{2})\bar{p}^2 - \epsilon\overline{U}(\bar{q})]$.

[d] For the case of BGK dynamics, $\overline{\rho}_{\bar{p},\rm EQ}(\bar{p}) = \hat{Z}_p^{-1}\exp[-(\frac{1}{2})\bar{p}^2]$, where $\overline{Z}_p = \int d\bar{p}\exp[-(\frac{1}{2})\bar{p}^2]$.

system phase space. For local models, such as Liouville and Fokker–Planck dynamics, $L(\Gamma,\Gamma') = L(\Gamma)\delta(\Gamma - \Gamma')$, where $L(\Gamma)$ is a differential operator (see Table II). For such cases, Eq. (4.3b) assumed the differential form

$$L(\Gamma)[\delta(\Gamma - \Gamma')\rho_{\rm EQ}(\Gamma')] = \rho_{\rm EQ}(\tilde{\Gamma})[L^{T}(\tilde{\Gamma})\delta(\tilde{\Gamma} - \tilde{\Gamma}')]. \tag{4.5}$$

The above form is similar to the version of detailed balance discussed by Haken,[6c] Risken,[5b,6b] and Stillman and Freed[6b] for generalized Fokker–Planck systems in detailed balance. An account of the implications of the results of these investigators is given at the end of this section.

The results given by Eqs. (4.3b) and (4.5) reveal that the universal dynamical constraint given by Eq. (3.8) is a universal operator relation that embodies detailed balance for both local and nonlocal globally linear classical dynamical models. In essence, we have shown that the above versions of detailed balance may be derived from the necessary and sufficient condition given by Eq. (3.8) for the stationarity of classical time correlation functions. To our knowledge, the concept of detailed balance has not been shown to emerge in such a fundamental way from basic principles. Usually detailed balance is simply a statement of commonly held intuitive notions about the behavior of a system in the state of equilibrium. Our results reveal that detailed balance is much more fundamental. Given this observation, it is our opinion that detailed balance should be regarded as a universal dynamical constraint as embodied in Eq. (3.8). Hence, we shall refer to Eq. (3.8) as the universal operator formulation of detailed balance.

If the transition operator $\hat{L}$ is invariant under the transformation given by Eq. (3.11), i.e., $\hat{L}_{\rm EQ} = \hat{L}$, the universal formulation of detailed balance given by Eq. (3.8) reduces to the operator relation

$$\hat{\tilde{L}} = \hat{L}^{T}. \tag{4.6}$$

In the classical phase space representation, the above symmetry relation assumes the form of a version of microscopic reversibility:

$$L(\tilde{\Gamma},\tilde{\Gamma}') = L^{T}(\Gamma,\Gamma') \tag{4.7a}$$

$$= L(\Gamma',\Gamma). \tag{4.7b}$$

The above results reveal that microscopic reversibility is also embodied in Eq. (3.8) and that it is a special case of detailed balance. Henceforth, we shall refer to Eq. (4.6) as the universal operator formulation of microscopic reversibility.

For the case of Liouville dynamics, $\hat{L}_{\rm EQ} = \hat{L}$ and $\tilde{L} = -\hat{L}$ (see Table II). Hence, the symmetry relation $\hat{L}^{T} = -\hat{L}$ must be satisfied in order for Liouville dynamics to be consistent with microscopic reversibility and more generally detailed balance. As we indicated earlier, the symmetry relation $\hat{L}^{T} = -\hat{L}$ applies for Liouville dynamics only when we are dealing with a closed system.

If Eq. (4.6) does indeed represent a universal operator formulation of microscopic reversibility, we should be able to use this symmetry relation to establish the usual formulations given in terms of conditional transition probabilities.[3] Making use of the relations

$$(\Gamma'|\exp(-\hat{L}t)|\Gamma) = (\Gamma|\exp(-\hat{L}^{T}t)|\Gamma')$$

and

$$(\Gamma'|\exp(\tilde{L}t)|\Gamma) = (\Gamma|\exp(\tilde{L}^{T})|\Gamma')$$

and the formal expressions given by Eqs. (2.6c) and (2.7c), we find with the aid of Eq. (4.6) that

$$P^{>}(\Gamma',t|\Gamma,0) = P^{>}(\tilde{\Gamma},t|\tilde{\Gamma}',0) \tag{4.8}$$

and

$$P^{<}(\Gamma',t|\Gamma,0) = P^{<}(\tilde{\Gamma},t|\tilde{\Gamma}',0). \tag{4.9}$$

It follows from Eqs. (2.5), (4.8), and (4.9) that the conditional transition probability $P(\Gamma',t|\Gamma,0)$ satisfies the symmetry relation

$$P(\Gamma',t|\Gamma,0) = P(\tilde{\Gamma},t|\tilde{\Gamma}',0). \tag{4.10}$$

Combining this result with Eq. (2.15), we obtain

$$P(\Gamma',t|\Gamma,0) = P(\Gamma,-t|\Gamma',0). \tag{4.11}$$

The usual approach[3] for establishing microscopic reversibility as described by Eqs. (4.10) and (4.11) is to employ complicated arguments based on causality and the time-reversal invariance of Hamilton's equations. Although this approach is useful, it only establishes sufficient conditions for the realization of microscopic reversibility as described by Eqs. (4.10) and (4.11). In sharp contrast to the usual approaches, we have established Eqs. (4.10) and (4.11) in a rather trivial fashion without appealing to any dynamical model and demonstrated that they are simply a consequence of a special case of the universal dynamical constraint given by Eq. (3.8). To our knowledge, Eqs. (4.10) and (4.11) have not been established before in such a simple and elegant fashion based solely on universal symmetry principles.

Now let us show that the universal dynamical constraint given by Eq. (3.8) leads to the formulation of detailed balance given in terms of joint probabilities, i.e.,[3,5,7a]

$$P(\Gamma,t|\Gamma',0)\rho_{\rm EQ}(\Gamma') = P(\tilde{\Gamma}',t|\tilde{\Gamma},0)\rho_{\rm EQ}(\tilde{\Gamma}), \tag{4.12}$$

where the equality $\rho_{\rm EQ}(\tilde{\Gamma}) = \rho_{\rm EQ}(\Gamma)$ is required by virtue of the initial condition $\delta(\Gamma - \Gamma')\rho_{\rm EQ}(\Gamma') = \theta(\tilde{\Gamma}' - \tilde{\Gamma})\rho_{\rm EQ}(\tilde{\Gamma})$.[6a,6c]

Making use of Eqs. (2.6c) and (2.7c), we can write the retarded and advanced components of the joint probability $P(\Gamma,t|\Gamma',0)\rho_{\rm EQ}(\Gamma')$ as

$$P^{>}(\Gamma,t|\Gamma',0)\rho_{\rm EQ}(\Gamma') = \theta(t)(\Gamma|\exp(-\hat{L}t)|\Gamma'\rho_{\rm EQ}) \tag{4.13}$$

and

$$P^{<}(\Gamma,t|\Gamma',0)\rho_{\rm EQ}(\Gamma') = \theta(-t)(\Gamma|\exp(\hat{\tilde{L}}t)|\Gamma'\rho_{\rm EQ}), \tag{4.14}$$

where the components of the dynamical vector $|\Gamma'\rho_{\rm EQ})$ are given by $(\Gamma|\Gamma'\rho_{\rm EQ}) = \delta(\Gamma - \Gamma')\rho_{\rm EQ}(\Gamma')$ in the classical phase space representation (see Table I).

With Eqs. (4.13) and (4.14) at our disposal, we can make use of the transformation given by Eq. (3.11) and the universal dynamical constraint given by Eq. (3.8) to write

$$P^{>}(\Gamma,t|\Gamma',0)\rho_{\rm EQ}(\Gamma') = P^{>}(\tilde{\Gamma}',t|\tilde{\Gamma},0)\rho_{\rm EQ}(\tilde{\Gamma}) \tag{4.15}$$

and

$$P^{<}(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=P^{<}(\tilde{\Gamma}',t\,|\tilde{\Gamma},0)\rho_{\rm EQ}(\tilde{\Gamma}). \tag{4.16}$$

The version of detailed balance given by Eq. (4.12) follows from the above symmetry relations and Eq. (2.5).

Making use of the conservation of probability relations

$$\int_{\mathscr{D}} d\Gamma(\Gamma|\exp(-\hat{L}t)=\int_{\mathscr{D}} d\Gamma(\Gamma|$$

for $t>0$ and

$$\int_{\mathscr{D}} d\Gamma(\Gamma|\exp(\tilde{L}t)=\int_{\mathscr{D}} d\Gamma(\Gamma|$$

for $t<0$ (see Table I), the relations $\hat{L}\,|\rho_{\rm EQ})=|0)$ and $\tilde{L}\,|\rho_{\rm EQ})=|0)$ obtained in Sec. IV A, and Eqs. (4.13) and (4.14), one can very easily establish that

$$\int_{\mathscr{D}} d\Gamma\, P^{>}(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma) \tag{4.17}$$

and

$$\int_{\mathscr{D}} d\Gamma'\, P^{>}(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma)$$

for $t>0$, and (4.18)

$$\int_{\mathscr{D}} d\Gamma\, P^{<}(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma') \tag{4.19}$$

and

$$\int_{\mathscr{D}} d\Gamma'\, P^{<}(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma)$$

for $t<0$. (4.20)

It follows from Eqs. (2.5) and (4.17)–(4.20) that the joint probability $P(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')$ possesses the properties

$$\int_{\mathscr{D}} d\Gamma\, P(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma') \tag{4.21}$$

and

$$\int_{\mathscr{D}} d\Gamma'\, P(\Gamma,t\,|\Gamma',0)\rho_{\rm EQ}(\Gamma')=\rho_{\rm EQ}(\Gamma). \tag{4.22}$$

The results given by Eqs. (4.12), (4.21), and (4.22) resemble the properties of the joint probabilities for so-called "coarse-grained" variables in the de Groot–Mazur treatment of detailed balance in their formulation of the statistical foundations of nonequilibrium thermodynamics.[3a] The de Groot–Mazur treatment of this problem is quite complicated, relies on the use of Hamilton's equations, and applies only to "coarse-grained" microcanonical ensembles described by reversible dynamics. In sharp contrast to the de Groot–Mazur treatment, we have established Eqs. (4.12), (4.21) and (4.22) in a rather trivial fashion without any reference to a specific dynamical model other than requiring that the dynamics conform to the universal operator relations embodying detailed balance and conservation of probability.

Starting with the argument that detailed balance is a physical property common to systems in thermal equilibrium and to those in more general stationary states described by a potential function, Graham and Haken[6a] used a version of detailed balance identical in form to Eq. (4.12) to derive a set of restrictive conditions (called potential conditions) on the drift and diffusion coefficients in generalized Fokker–Planck equations. They showed that this set of conditions ensure that a Fokker–Planck equation satisfies detailed balance and guarantee that it is always possible to explicitly determine the stationary solution of a Fokker–Planck equation by quadratures.

The results of Graham and Haken[6a,6c] were further elucidated by Risken.[5b,6b] More specifically, Risken[6b] established that a version of detailed balance, identical in form to Eq. (4.5) represents a necessary and sufficient condition for detailed balance as described by Eq. (4.12) for the case of local generalized Fokker–Planck systems. Furthermore, Risken[6b] showed that this localized version of detailed balance provides a simple starting point for deriving the above-mentioned Graham–Haken potential conditions.

The utility of the Graham–Haken–Risken treatment[6] of detailed balance in stochastic modeling has been demonstrated by Stillman and Freed.[6d] In particular, these investigators showed that the Graham–Haken potential conditions[6] could be employed as a vehicle for correcting Fokker–Planck equations[6d] that fail to describe relaxation to the correct stationary state due to their violation of detailed balance.

C. Generalized symmetry relations

Now let us show that the universal dynamical constraint given by Eq. (3.8) implies the existence of certain generalized symmetry relations for $C_{A,B}(t)$,$C^{>}_{A,B}(t)$,$C^{<}_{A,B}(t)$, $\mathscr{C}^{>}_{A,B}(z)$ [Laplace transform of $C^{>}_{A,B}(t)$], and $\mathscr{C}^{F}_{A,B}(i\omega)$ [Fourier transform of $C_{A,B}(t)$].

The symmetry properties of the retarded and advanced components of the time correlation function $C_{A,B}(t)$ may be established by starting with Eqs. (3.6b) and (3.7b) and adopting a procedure similar to the one used for establishing Eqs. (4.15) and (4.16). Taking this approach, we obtain

$$C^{>}_{A,B}(t)=C^{>}_{\tilde{B},\tilde{A}}(t) \tag{4.23}$$

and

$$C^{<}_{A,B}(t)=C^{<}_{\tilde{B},\tilde{A}}(t). \tag{4.24}$$

It follows from the above relations and Eq. (3.2) that the time correlation function $C_{A,B}(t)$ possesses the symmetry

$$C_{A,B}(t)=C_{\tilde{B},\tilde{A}}(t). \tag{4.25}$$

Equations (3.2), (3.6b), and (3.7b) imply the following additional symmetries for $C^{>}_{A,B}(t)$, $C^{<}_{B,A}(t)$, and $C_{A,B}(t)$:

$$C^{>}_{A,B}(t)=C^{<}_{\tilde{A},\tilde{B}}(-t), \tag{4.26}$$

$$C^{<}_{A,B}(t)=C^{>}_{\tilde{A},\tilde{B}}(-t), \tag{4.27}$$

and

$$C_{A,B}(t)=C_{\tilde{A},\tilde{B}}(-t). \tag{4.28}$$

Note that the symmetries given by Eqs. (4.25) and (4.28) are consistent with the stationarity condition given by Eq. (3.9).

It is evident from Eq. (4.23) that the Laplace transform

$\mathscr{C}^{>}_{A,B}(z)$ of the retarded component $C^{>}_{A,B}(t)$ of the time correlation function $C_{A,B}(t)$ satisfies the symmetry relation

$$\mathscr{C}^{>}_{A,B}(z) = \mathscr{C}^{>}_{\tilde{B},\tilde{A}}(z). \tag{4.29}$$

The stationarity condition given by Eq. (3.9) and the symmetry relation given by Eq. (4.25) may be used to establish the following symmetry relations for the Fourier transform $\mathscr{C}^{F}_{A,B}(i\omega)$ of the time correlation function $C_{A,B}(t)$:

$$\mathscr{C}^{F}_{A,B}(i\omega) = \mathscr{C}^{F}_{\tilde{B},\tilde{A}}(i\omega) \tag{4.30}$$

and

$$\mathscr{C}^{F}_{A,B}(i\omega) = \mathscr{C}^{F}_{B,A}(-i\omega). \tag{4.31}$$

Clearly,

$$\mathscr{C}^{F}_{\tilde{B},\tilde{A}}(i\omega) = \mathscr{C}^{F}_{B,A}(-i\omega). \tag{4.32}$$

It should be evident that all of the symmetry relations given by Eqs. (4.23)–(4.32) are a consequence of the universal dynamical constraint given by Eq. (3.8). Hence, they have universal applicability for all acceptable globally linear classical dynamical models. Clearly, the violation of these symmetry relations is a symptom of the use of an unacceptable model that violates Eq. (3.8). If this is indeed the case, the stationarity condition given by Eq. (3.9) is also violated.

For cases in which the dynamical variables A and B possess definite time-reversal parity, the generalized symmetry relations given by Eqs. (4.25), (4.29), (4.30), and (4.32) assume the well-known forms[13]

$$C_{A,B}(t) = \lambda_A \lambda_B C_{B,A}(t), \tag{4.33}$$

$$\mathscr{C}^{>}_{A,B}(z) = \lambda_A \lambda_B \mathscr{C}^{>}_{B,A}(z), \tag{4.34}$$

$$\mathscr{C}^{F}_{A,B}(i\omega) = \lambda_A \lambda_B \mathscr{C}^{F}_{B,A}(i\omega), \tag{4.35}$$

and

$$\mathscr{C}^{F}_{A,B}(i\omega) = \lambda_A \lambda_B \mathscr{C}^{F}_{A,B}(-i\omega) \tag{4.36}$$

usually associated with globally reversible systems, where $\lambda_A\,[\lambda_B]$ is the time-reversal parity of $A[B]$.

Of course, the reader should realize that the symmetry relations given by Eqs. (4.33)–(4.36) and the generalized symmetry relations given by Eqs. (4.23)–(4.32) apply to both reversible and irreversible systems. A number of examples that conform to these symmetry relations may be found in our papers on dual Lanczos transformation theory.[1,2,8,12]

Usual approaches[13] for establishing the symmetry relations given by Eqs. (4.33)–(4.36) for the case of reversible systems either rely on traditional time-reversal transformation methods, such as those utilizing arguments based on the time-reversal invariance of Hamilton's equations, or appeal to the formulation of microscopic reversibility or detailed balance given by Eqs. (4.10)–(4.12). For the case of irreversible systems, the symmetry relations given by Eqs. (4.33) and (4.34) have been established by making use of the version of detailed balance given by Eq. (4.12).[7a]

Although the aforementioned approaches for establishing Eqs. (4.33)–(4.36) have been useful, they are generally complicated and model dependent. Moreover, these approaches have only led to sufficient conditions for the applicability of Eqs. (4.33)–(4.36). In sharp contrast to these approaches, we have established the generalized symmetry relations given by Eqs. (4.23)–(4.32), which include Eqs. (4.33)–(4.36) as special cases, in a rather trivial fashion without any reference to a specific model and shown them to be simply a consequence of the universal dynamical constraint given by Eq. (3.8). Also, we have already shown that the versions of microscopic reversibility and detailed balance that have actually served as a starting point in the proof of Eqs. (4.33)–(4.36) are also consequences of Eq. (3.8).

V. AN ILLUSTRATIVE APPLICATION

Apart from elucidating some fundamental symmetries of classical dynamical systems, the theory given in the preceding sections has the advantage of providing a simple model independent framework for treating classical time correlation functions via the extraction and utilization of dynamically embedded information.[1,2] Let us proceed to demonstrate this by exploiting the mathematical apparatus of dual Lanczos transformation theory[1,2,8,12] to determine the retarded and advanced components of the elements of the correlation matrices for first and second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.[1,8b,8c,9] Also, we wish to obtain the Laplace transforms[8c] of the retarded components of the time correlation functions and the Fourier transforms[1] of the full correlation functions.

As we have demonstrated elsewhere,[8b] the correlation matrices for first and second moment coordinate and momentum fluctuations are important not only for pedagogical reasons but also because they have an important bearing on problems in nonlinear dynamics and represent the spontaneous fluctuations that drive the temporal evolution of the noise filtered dynamical variables $\Delta q(t)$, $\Delta p(t)$, $\Delta q^2(t)$, $\Delta qp(t)$, and $\Delta p^2(t)$ for the Brownian harmonic oscillator, where $\Delta A(t) = A(t) - \langle A \rangle_{EQ}$ and p and q denote the momentum and coordinate, respectively. It should be evident that the dynamical variables $\Delta p(t)$ and $\Delta q(t)$ characterize the temporal evolution of the noise filtered trajectory $[p(t),q(t)]$, while the dynamical variables $\Delta q^2(t)$, $\Delta qp(t)$, and $\Delta p^2(t)$ characterize the noise filtered square displacements of the Brownian harmonic oscillator and its energy relaxation.

The correlation matrices for first and second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator are as follows:[8b]

$$\mathbf{C}^{(1)}(t) = \begin{pmatrix} \ll \Delta q(t)\Delta q(0) \gg_{EQ} & \ll \Delta q(t)\Delta p(0) \gg_{EQ} \\ \ll \Delta p(t)\Delta q(0) \gg_{EQ} & \ll \Delta p(t)\Delta p(0) \gg_{EQ} \end{pmatrix} \tag{5.1}$$

and

$$\mathbf{C}^{(2)}(t) = \begin{pmatrix} \ll \Delta q^2(t)\Delta q^2(0) \gg_{EQ} & \ll \Delta q^2(t)\Delta qp(0) \gg_{EQ} & \ll \Delta q^2(t)\Delta p^2(0) \gg_{EQ} \\ \ll \Delta qp(t)\Delta q^2(0) \gg_{EQ} & \ll \Delta qp(t)\Delta qp(0) \gg_{EQ} & \ll \Delta qp(t)\Delta p^2(0) \gg_{EQ} \\ \ll \Delta p^2(t)\Delta q^2(0) \gg_{EQ} & \ll \Delta p^2(t)\Delta qp(0) \gg_{EQ} & \ll \Delta p^2(t)\Delta p^2(0) \gg_{EQ} \end{pmatrix}. \tag{5.2}$$

TABLE III. Retarded components of the elements of the correlation matrix for first moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Retarded component $C^{>}_{A,B}(t)$	Type of eigenvalues[a,b]	Explicit form
$C^{>}_{\Delta q,\Delta q}(t) =$ $\theta(t)\langle\Delta q(t)\Delta q(0)\rangle_{EQ}$	2 distinct	$\theta(t)\exp[-(\eta/2)t]\{\cosh[(\frac{1}{2})(\eta^2-4)^{1/2}t]+[\eta/(\eta^2-4)^{1/2}]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]\}$
	1 of multiplicity 2	$\theta(t)(1+t)\exp(-t)$
$C^{>}_{\Delta q,\Delta p}(t) =$ $\theta(t)\langle\Delta q(t)\Delta p(0)\rangle_{EQ}$	2 distinct	$\theta(t)[2/(\eta^2-4)^{1/2}]\exp[-(\eta/2)t]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]$
	1 of multiplicity 2	$\theta(t)t\exp(-t)$
$C^{>}_{\Delta p,\Delta q}(t) =$ $\theta(t)\langle\Delta p(t)\Delta q(0)\rangle_{EQ}$	2 distinct	$-\theta(t)[2/(\eta^2-4)^{1/2}]\exp[-(\eta/2)t]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]$
	1 of multiplicity 2	$-\theta(t)t\exp(-t)$
$C^{>}_{\Delta p,\Delta p}(t) =$ $\theta(t)\langle\Delta p(t)\Delta p(0)\rangle_{EQ}$	2 distinct	$\theta(t)\exp[-(\eta/2)t]\{\cosh[(\frac{1}{2})(\eta^2-4)^{1/2}t]-[\eta/(\eta^2-4)^{1/2}]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]\}$
	1 of multiplicity 2	$\theta(t)(1-t)\exp(-t)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).
[b] $\eta\neq 2$ for the case of two distinct eigenvalues. $\eta=2$ for the case of 1 eigenvalue of multiplicity 2. See Ref. 8(b).

In Eqs. (5.1) and (5.2) p and q are the dimensionless momentum and coordinate, respectively, for the Brownian harmonic oscillator. The time t is also dimensionless. Hereafter, it should be understood that we are working in dimensionless units. For additional details, see Ref. 8(b).

The double bracket notation $\ll A(t)B(0)\gg_{EQ}$ in Eqs. (5.1) and (5.2) for the time correlation functions has been used to indicate that these time correlation functions are of the type discussed in Sec. III for which the propagation of the fluctuations is described in both the forward and backward time directions. The reader should not confuse $\ll A(t)B(0)\gg_{EQ}$ with $\langle A(t)B(0)\rangle_{EQ}$. The formal connection between these time correlation functions is given by Eqs. (3.17a) and (3.17b).

TABLE IV. Advanced components of the elements of the correlation matrix for first moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Advanced component $C^{<}_{A,B}(t)$	Type of eigenvalues[a,b]	Explicit form
$C^{<}_{\Delta q,\Delta q}(t) =$ $\theta(-t)\langle\Delta q(-t)\Delta q(0)\rangle_{EQ}$	2 distinct	$\theta(t)\exp[(\eta/2)t]\{\cosh[(\frac{1}{2})(\eta^2-4)^{1/2}t]-[\eta/(\eta^2-4)^{1/2}]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]\}$
	1 of multiplicity 2	$\theta(-t)(1-t)\exp(t)$
$C^{<}_{\Delta q,\Delta p}(t) =$ $-\theta(-t)\langle\Delta q(-t)\Delta p(0)\rangle_{EQ}$	2 distinct	$\theta(-t)[2/(\eta^2-4)^{1/2}]\exp[(\eta/2)t]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]$
	1 of multiplicity 2	$\theta(-t)t\exp(t)$
$C^{<}_{\Delta p,\Delta q}(t) =$ $-\theta(-t)\langle\Delta p(-t)\Delta q(0)\rangle_{EQ}$	2 distinct	$-\theta(-t)[2/(\eta^2-4)^{1/2}]\exp[(\eta/2)t]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]$
	1 of multiplicity 2	$-\theta(-t)t\exp(t)$
$C^{<}_{\Delta p,\Delta p}(t) =$ $\theta(-t)\langle\Delta p(-t)\Delta p(0)\rangle_{EQ}$	2 distinct	$\theta(-t)\exp[(\eta/2)t]\{\cosh[(\frac{1}{2})(\eta^2-4)^{1/2}t]+[\eta/(\eta^2-4)^{1/2}]\sinh[(\frac{1}{2})(\eta^2-4)^{1/2}t]\}$
	1 of multiplicity 2	$\theta(-t)(1+t)\exp(t)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).
[b] $\eta\neq 2$ for the case of two distinct eigenvalues. $\eta=2$ for the case of 1 eigenvalue of multiplicity 2. See Ref. 8(b).

TABLE V. Retarded components of the elements of the correlation matrix for second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Retarded component $C^{>}_{A,B}(t) =$	Type of eigenvalues[a,b]	Explicit form
$C^{>}_{\Delta q^2,\Delta q^2}(t) =$	3 distinct	$2\theta(t)\exp(-\eta t)\{[(\eta^2-2)/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [\eta/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [2/(\eta^2-4)]\}$
$\theta(t)\langle\Delta q^2(t)\Delta q^2(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)(1+t)^2\exp(-2t)$
$C^{>}_{\Delta q^2,\Delta qp}(t) =$	3 distinct	$2\theta(t)\exp(-\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$\theta(t)\langle\Delta q^2(t)\Delta qp(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)t(1+t)\exp(-2t)$
$C^{>}_{\Delta q^2,\Delta p^2}(t) =$	3 distinct	$\theta(t)[4/(\eta^2-4)]\exp(-\eta t)\{-1+\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(t)\langle\Delta q^2(t)\Delta p^2(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)t^2\exp(-2t)$
$C^{>}_{\Delta qp,\Delta q^2}(t) =$	3 distinct	$-2\theta(t)\exp(-\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$\theta(t)\langle\Delta qp(t)\Delta q^2(0)\rangle_{EQ}$	1 of multiplicity 3	$-2\theta(t)t(1+t)\exp(-2t)$
$C^{>}_{\Delta qp,\Delta qp}(t) =$	3 distinct	$\theta(t)[1/(\eta^2-4)]\exp(-\eta t)\{\eta^2-4\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(t)\langle\Delta qp(t)\Delta qp(0)\rangle_{EQ}$	1 of multiplicity 3	$\theta(t)(1-2t^2)\exp(-2t)$
$C^{>}_{\Delta qp,\Delta p^2}(t) =$	3 distinct	$-2\theta(t)\exp(-\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] - [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$\theta(t)\langle\Delta qp(t)\Delta p^2(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)t(1-t)\exp(-2t)$
$C^{>}_{\Delta p^2,\Delta q^2}(t) =$	3 distinct	$\theta(t)[4/(\eta^2-4)]\exp(-\eta t)\{-1+\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(t)\langle\Delta p^2(t)\Delta q^2(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)t^2\exp(-2t)$
$C^{>}_{\Delta p^2,\Delta qp}(t) =$	3 distinct	$2\theta(t)\exp(-\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] - [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$\theta(t)\langle\Delta p^2(t)\Delta qp(0)\rangle_{EQ}$	1 of multiplicity 3	$-2\theta(t)t(1-t)\exp(-2t)$
$C^{>}_{\Delta p^2,\Delta p^2}(t) =$	3 distinct	$2\theta(t)\exp(-\eta t)\{[(\eta^2-2)/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [2/(\eta^2-4)]\}$
$\theta(t)\langle\Delta p^2(t)\Delta p^2(0)\rangle_{EQ}$	1 of multiplicity 3	$2\theta(t)(1-t)^2\exp(-2t)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).
[b] $\eta \neq 2$ for the case of 3 distinct eigenvalues. $\eta = 2$ for the case of 1 eigenvalue of multiplicity 3. See Ref. 8(b).

One can readily determine the retarded [advanced] component $C^{>}_{A,B}(t)\,[C^{<}_{A,B}(-t)]$ of each time correlation function $C_{A,B}(t)$ in Eqs. (5.1) and (5.2) for $t>0$ by first casting $C^{>}_{A,B}(t)\,[C^{<}_{A,B}(-t)]$ into the form of Eq. (3.6b) [Eq. (3.7b)] and subsequently making use of the concept of extraction and utilization of dynamically embedded information[1,2] from dual Lanczos transformation theory.[1,2,8] $C^{<}_{A,B}(t)$ is obtained from $C^{<}_{A,B}(-t)$ by simply replacing t with $-t$. The results for the retarded and advanced components obtained by this procedure are summarized in Tables

TABLE VI. Advanced components of the elements of the correlation matrix for second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Advanced component $C^{<}_{A,B}(t)$	Type of eigenvalues[a,b]	Explicit form
$C^{<}_{\Delta q^2,\Delta q^2}(t) =$	3 distinct	$2\theta(-t)\exp(\eta t)\{[(\eta^2-2)/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [2/(\eta^2-4)]\}$
$\theta(-t)\langle\Delta q^2(-t)\Delta q^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(-t)(1-t)^2\exp(2t)$
$C^{<}_{\Delta q^2,\Delta qp}(t) =$	3 distinct	$-2\theta(-t)\exp(\eta t)\{[\eta/(\eta^4-4]\cosh[(\eta^2-4)^{1/2}t] - [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$-\theta(-t)\langle\Delta q^2(-t)\Delta qp(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(-t)t(1-t)\exp(2t)$
$C^{<}_{\Delta q^2,\Delta p^2}(t) =$	3 distinct	$\theta(-t)[4/(\eta^2-4)]\exp(\eta t)\{-1+\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(-t)\langle\Delta q^2(-t)\Delta p^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(-t)t^2\exp(2t)$
$C^{<}_{\Delta qp,\Delta q^2}(t) =$	3 distinct	$2\theta(-t)\exp(\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] - [1/(\eta^2-4)]^{1/2}\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$-\theta(-t)\langle\Delta qp(-t)\Delta q^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$-2\theta(-t)t(1-t)\exp(2t)$
$C^{<}_{\Delta qp,\Delta qp}(t) =$	3 distinct	$\theta(-t)[1/(\eta^2-4)]\exp(\eta t)\{\eta^2-4\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(-t)\langle\Delta qp(-t)\Delta qp(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$\theta(-t)(1-2t^2)\exp(2t)$
$C^{<}_{\Delta qp,\Delta p^2}(t) =$	3 distinct	$2\theta(-t)\exp(\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$-\theta(-t)\langle\Delta qp(-t)\Delta p^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(t)t(1+t)\exp(2t)$
$C^{<}_{\Delta p^2,\Delta q^2}(t) =$	3 distinct	$\theta(-t)[4/(\eta^2-4)]\exp(\eta t)\{-1+\cosh[(\eta^2-4)^{1/2}t]\}$
$\theta(-t)\langle\Delta p^2(-t)\Delta q^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(-t)t\exp(2t)$
$C^{<}_{\Delta p^2,\Delta qp}(t) =$	3 distinct	$-2\theta(-t)\exp(\eta t)\{[\eta/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [1/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [\eta/(\eta^2-4)]\}$
$-\theta(-t)\langle\Delta p^2(-t)\Delta qp(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$-2\theta(-t)t(1+t)\exp(2t)$
$C^{<}_{\Delta p^2,\Delta p^2}(t) =$	3 distinct	$2\theta(-t)\exp(\eta t)\{[(\eta^2-2)/(\eta^2-4)]\cosh[(\eta^2-4)^{1/2}t] + [\eta/(\eta^2-4)^{1/2}]\sinh[(\eta^2-4)^{1/2}t] - [2/(\eta^2-4)]\}$
$\theta(-t)\langle\Delta p^2(-t)\Delta p^2(0)\rangle_{\mathrm{EQ}}$	1 of multiplicity 3	$2\theta(-t)(1+t)^2\exp(2t)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).
[b] $\eta \neq 2$ for the case of 3 distinct eigenvalues. $\eta = 2$ for the case of 1 eigenvalue of multiplicity 3. See Ref. 8(b).

III–VI.[14] The full time correlation function $C_{A,B}(t)$ is obtained by simply adding the retarded and advanced components [see Eq. (3.2)] in these tables. Note that the results displayed in Tables III–VI conform to the symmetry relations given by Eqs. (4.23), (4.24), (4.26), and (4.27). Moreover, the full time correlation functions assembled from these results conform to the symmetry relations given by Eqs. (3.9), (4.25), and (4.28) [see Eq. (3.2)].

The Laplace transform [see Eq. (3.6b)]

$$\mathscr{C}^{>}_{A,B}(z) = (A\,|(z\hat{I}+\hat{L})^{-1}|B\rho_{\mathrm{EQ}}) \tag{5.3}$$

TABLE VII. Laplace transforms of the retarded components of the elements of the correlation matrix for first moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Laplace transform $\mathscr{C}^{>}_{A,B}(z)$	Explicit form[a]
$\mathscr{C}^{>}_{\Delta q,\Delta q}(z)$	$a^{>}_{0,0}(z)$
$\mathscr{C}^{>}_{\Delta q,\Delta p}(z)$	$-z[a^{>}_{0,0}(z)-(1/z)]$
$\mathscr{C}^{>}_{\Delta p,\Delta q}(z)$	$z[a^{>}_{0,0}(z)-(1/z)]$
$\mathscr{C}^{>}_{\Delta p,\Delta p}(z)$	$-z^2[a^{>}_{0,0}(z)-(1/z)]$

[a] $a^{>}_{0,0}(z)=[(z+\eta)/(z^2+\eta z+1)]$, where η is the dimensionless friction coefficient defined in Ref. 8(b).

TABLE IX. Fourier transforms of the elements of the correlation matrix for first moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Fourier transform $\mathscr{C}^{F}_{A,B}(i\omega)$	Explicit form[a]
$\mathscr{C}^{F}_{\Delta q,\Delta q}(i\omega)$	$2\eta/[(1-\omega^2)^2+\omega^2\eta^2]$
$\mathscr{C}^{F}_{\Delta q,\Delta p}(i\omega)$	$-i\omega\mathscr{C}^{F}_{\Delta q,\Delta q}(i\omega)$
$\mathscr{C}^{F}_{\Delta p,\Delta q}(i\omega)$	$i\omega\mathscr{C}^{F}_{\Delta q,\Delta q}(i\omega)$
$\mathscr{C}^{F}_{\Delta p,\Delta p}(i\omega)$	$\omega^2\mathscr{C}^{F}_{\Delta q,\Delta q}(i\omega)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).

of the retarded component $C^{>}_{A,B}(t)$ of each of the time correlation functions in Eqs. (5.1) and (5.2) may also be readily determined via the extraction and utilization of dynamically embedded information.[1,2] Following such a procedure, we are led to the results displayed in Tables VII and VIII.[15] Note that these results conform to the symmetry relation given by Eq. (4.29).

Finally, the Fourier transform $\mathscr{C}^{F}_{A,B}(i\omega)$ of each time correlation function $C_{A,B}(t)$ in Eqs. (5.1) and (5.2) may be determined by writing $\mathscr{C}^{F}_{A,B}(i\omega)$ in the form [see Eq. (3.5b)]

$$\mathscr{C}^{F}_{A,B}(i\omega)=\lim_{\epsilon\to 0^+}\{(A\,|[(i\omega+\epsilon)\hat{I}+\hat{L}\,]^{-1}|B\rho_{\mathrm{EQ}})+(\tilde{A}\,|[(-i\omega+\epsilon)\hat{I}+\hat{L}\,]^{-1}|\tilde{B}\rho_{\mathrm{EQ}})\} \tag{5.4}$$

and subsequently exploiting the concept of extraction and utilization of dynamically embedded information.[1,2] Such a procedure leads to the results displayed in Tables IX and X.[16] Note that these results conform to the symmetry relations given by Eqs. (4.30)–(4.32).

VI. CONCLUDING REMARKS

We rigorously established from basic principles a universal dynamical constraint for globally linear classical dynamical models intended to describe the execution of spontaneous fluctuations about a stationary state. It was shown that this constraint arises from the requirement of stationarity and represents a necessary and sufficient condition for its realization for all time correlation functions associated with a given globally linear classical dynamical system. Since stationarity is a physical requirement that must be satisfied, the constraint is of universal character with applicability to all globally linear classical dynamical models. If the constraint

TABLE VIII. Laplace transforms of the retarded components of the elements of the correlation matrix for second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Laplace transform $\mathscr{C}^{>}_{A,B}(z)$	Explicit form[a]
$\mathscr{C}^{>}_{\Delta q^2,\Delta q^2}(z)$	$2a^{>}_{0,0}(z)$
$\mathscr{C}^{>}_{\Delta q^2,\Delta qp}(z)$	$-z[a^{>}_{0,0}(z)-(1/z)]$
$\mathscr{C}^{>}_{\Delta q^2,\Delta p^2}(z)$	$(z^2+\eta z+2)[a^{>}_{0,0}(z)-(z+\eta)/(z^2+\eta z+2)]$
$\mathscr{C}^{>}_{\Delta qp,\Delta q^2}(z)$	$z[a^{>}_{0,0}(z)-(1/z)]$
$\mathscr{C}^{>}_{\Delta qp,\Delta qp}(z)$	$-(z^2/2)[a^{>}_{0,0}(z)-(1/z)]$
$\mathscr{C}^{>}_{\Delta qp,\Delta p^2}(z)$	$(\frac{1}{2})\{(z^3+\eta z^2+2z)[a^{>}_{0,0}(z)-(z+\eta)/(z^2+\eta z+2)]\}$
$\mathscr{C}^{>}_{\Delta p^2,\Delta q^2}(z)$	$(z^2+\eta z+2)[a^{>}_{0,0}(z)-(z+\eta)/(z^2+\eta z+2)]$
$\mathscr{C}^{>}_{\Delta p^2,\Delta qp}(z)$	$-(\frac{1}{2})\{(z^3+\eta z^2+2z)[a^{>}_{0,0}(z)-(z+\eta)/(z^2+\eta z+2)]\}$
$\mathscr{C}^{>}_{\Delta p^2,\Delta p^2}(z)$	$(\frac{1}{2})(z^2+\eta z+2)^2[a^{>}_{0,0}(z)-(z+\eta)/(z^2+\eta z+2)]$

[a] $a^{>}_{0,0}(z)=[z^2+3\eta z+2(\eta^2+1)]/[z^3+3\eta z^2+2(\eta^2+2)z+4\eta]$, where η is the dimensionless friction coefficient defined in Ref. 8(b).

TABLE X. Fourier transforms of the elements of the correlation matrix for second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.

Fourier transform $\mathscr{C}^F_{A,B}(i\omega)$	Explicit form[a]
$\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$	$8\eta\{[\omega^2+4(\eta^2+1)]/\{\eta^2(4-3\omega^2)^2+\omega^2[2(\eta^2+2)-\omega^2]^2\}$
$\mathscr{C}^F_{\Delta q^2,\Delta qp}(i\omega)$	$-(i\omega/2)\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta q^2,\Delta p^2}(i\omega)$	$\{(4-3\omega^2)/[4(\eta^2+1)+\omega^2]\}\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta qp,\Delta q^2}(i\omega)$	$(i\omega/2)\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta qp,\Delta qp}(i\omega)$	$(\omega^2/4)\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta qp,\Delta p^2}(i\omega)$	$\{i\omega(4-3\omega^2)/\{2[\omega^2+4(\eta^2+1)]\}\}\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta p^2,\Delta q^2}(i\omega)$	$\{(4-3\omega^2)/[4(\eta^2+1)+\omega^2]\}\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta p^2,\Delta qp}(i\omega)$	$-\{i\omega(4-3\omega^2)/\{2[\omega^2+4(\eta^2+1)]\}\}\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$
$\mathscr{C}^F_{\Delta p^2,\Delta p^2}(i\omega)$	$\{[(4-3\omega^2)+\omega^2(\omega^2+\eta^2)]/[\omega^2+4(\eta^2+1)]\}\mathscr{C}^F_{\Delta q^2,\Delta q^2}(i\omega)$

[a] η is the dimensionless friction coefficient defined in Ref. 8(b).

is not satisfied, stationarity and other symmetries arising from it will be violated for some or perhaps all dynamical variables.

It was shown that the universal dynamical constraint obtained by us (i) imposes restrictions on the symmetry of the transition operator appearing in the global propagator for a system; (ii) coupled with the conservation of probability implies that the equilibrium distribution is stationary with respect to the global dynamics, i.e., both the retarded and advanced dynamics of a system; (iii) represents a universal operator relation that embodies detailed balance and microscopic reversibility, giving rise to their traditional formulations for both local and nonlocal dynamical models; and (iv) implies the existence of certain generalized symmetry relations for time correlation functions and their Laplace and Fourier transforms that are applicable to both reversible and irreversible dynamical systems.

Apart from elucidating some fundamental symmetries of classical dynamical systems, the reported theory has the advantage of providing a simple model independent framework for treating classical time correlation functions via the extraction and utilization of dynamically embedded information.[1,2] This was demonstrated in a concrete way by exploiting the mathematical apparatus of dual Lanczos transformation theory[1,2,8,12] to determine the advanced and retarded components of the elements of the correlation matrices for the first and second moment coordinate and momentum fluctuations for the Brownian harmonic oscillator.[1,8b,c,9] We also obtained the Laplace transforms[8c] of the retarded components of the time correlations functions and the Fourier transforms[1] of the full time correlations functions. The results obtained were shown to conform to the symmetry relations implied by the universal operator formulation of detailed balance. This is a consequence of the fact that dual Lanczos transformation theory[1,2,8,12] works with dynamically invariant subspaces embedded with all of the pertinent dynamical information in spite of the use of a subdynamics of the global dynamics.[2]

Before concluding, we should remark that none of the approaches given by Mori,[17] Diestler,[18] Dupuis,[19] Lado,[20] Grigolini,[21] and Freed[22] are able to handle the problem of determining all of the results displayed in Tables III–X. As we have discussed at length many times before[1,2,8,12] all of these approaches suffer from different intrinsic limitations and represent special limiting cases of dual Lanczos transformation theory. The applicability of the approaches of Mori,[17] Diestler,[18] Dupuis,[19] Lado,[20] Grigolini,[21] and Freed[22] is at best limited to the determination of a single autocorrelation function for a restricted class of dynamical systems. Even for the problem of determining the Fourier transform of an autocorrelation function for an irreversible system and a cross-correlation function for a reversible or irreversible system these approaches have difficulties as a result of their intrinsic limitations and lack of a proper treatment of the retarded and advanced dynamics of a system.

Given that the Brownian harmonic oscillator has served and continues to serve as a prototype model system in nonequilibrium statistical mechanics,it is our opinion that any approach intended to provide an adequate framework for treating and understanding spectral and temporal properties of dynamical systems must at the very minimum be able to deal with the spectral and temporal properties of the Brownian harmonic oscillator. In this respect, all of the approaches given by Mori,[17] Diestler,[18] Dupuis,[19] Lado,[20] Grigolini,[21] and Freed[22] fail. In sharp contrast, the theory reported in this paper coupled with dual Lanczos transformation theory[1,2,8,12] is able to deal with the Brownian harmonic oscillator analytically in a rather trivial way and shows much promise in being able to handle more complicated systems.[12]

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Infrared singularities and breaking of the Poincaré group: The massless dipole field

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A four-dimensional quantum field theory model is studied that exhibits infrared singularities expected to occur in realistic models of confinement. The Fock–Hilbert–Krein structure associated with the model in a local and covariant formulation is constructed and its unconventional features, like the existence of translationally invariant field operators and states (other than the vacuum), the implementation of the symmetries, etc., are discussed. Also, a canonical quantization of the model which improves the existing ones is derived. Finally, it is shown that the infrared singularities are responsible of the breaking of the Poincaré group in every nontrivial physical space; two explicit examples of possible physical spaces are constructed and it is shown that they have the same gauge invariant content.

I. INTRODUCTION

The aim of the present paper is to provide a rigorous treatment of the dipole field model, that is a Hermitian scalar field satisfying the equation

$$\Box^2\phi = 0, \quad \Box = \partial^\mu\partial_\mu. \tag{1.1}$$

The motivations for such analysis are several. This model attracted the interest of theoretical physicists already in the 1950s under the influence of the debated paper of Källen and Pauli on the Lee model.[1–3] A revival of interest in the model came with the advent of gauge theories and this because the Fourier transform of the two-point function of the dipole field has a $\delta'(p^2)$ singularity, $p^2 = p^\mu p_\mu$. This singularity is the quantum field theory (QFT) version of the linearly growing potential believed a crucial feature of the quark–antiquark interaction.[4] Besides, it has been shown that the breaking of the gauge symmetry in the Abelian Higgs model requires, in local gauges, this kind of singularity.[5,6] Other classes of models that have a dipole field as a building block are the purely gauge QED,[7] the conformally invariant models,[8,9] and the supersymmetric models. From a general point of view, the model can be regarded as a simple prototype of a four-dimensional quantum field theory exhibiting infrared singularities of the confining type,[10] which are not compatible with the axiom of positivity.[11] Since the lack of positivity is an unavoidable feature of gauge quantum field theories when treated in local renormalizable gauges,[12] a rigorous treatment of this model will shed light on those general mathematical structures characterizing nonpositive QFT's in the Wightman framework.

Finally, a further motivation for a revisitation of this model is that the previous treatments are not completely satisfactory. The main open problems are: (1) a clear identification of the Hilbert space of states associated to the Wightman functions of this model; (2) the existence of translationally invariant states other than the vacuum state (i.e., the essential uniqueness of the vacuum); (3) the symmetry breaking problem in the model; (4) the possible identification of the physical space and the physical interpretation of the model; and (5) the justification of a canonical quantization of the field in a positive space.

As we will see, our results will significantly improve (actually in most of the cases correct) the previous treatments. The point is that, as emphasized in Refs. 10 and 13, the structural questions concerning an indefinite metric QFT cannot be correctly posed and answered without making reference to a Hilbert space realization of the model.

The starting point of the following discussion of the dipole field is a set of local and covariant Wightman functions that satisfy the weak spectral condition. The lack of positivity implies that the reconstruction theorem[10,11] yields only a linear space $\mathscr{D}$ endowed with a sesquilinear form $\langle\ ,\ \rangle$. To obtain a Hilbert space, it is necessary to introduce in $\mathscr{D}$ a Hilbert topology compatible with the intrinsic indefinite product $\langle\ ,\ \rangle$. There are, of course, many possible ways to introduce a Hilbert structure in $\mathscr{D}$, but the most interesting cases are given by those structures that are maximal, i.e., not properly contained in any other compatible Hilbert structure. In this case, the metric operator, η, which represents the sesquilinear form $\langle\ .\ \rangle$, has the property that $\eta^2 = 1$ and the corresponding Hilbert space is a Krein space.[14]

In Sec. II, we will construct a Hilbert–Krein structure associated with the dipole field; we will show that the Hilbert representation space K of the theory contains vectors (different from the vacuum) that are invariant under the Poincaré group (infrared states); the vacuum is, however, essentially unique,[10] i.e., there is no strictly positive (with respect to $\langle\ ,\ \rangle$ subspace of K invariant under translations, whose dimension is greater than 1. The infrared states have an interesting counterpart in the strong closure of the local field algebra: Indeed, this closure includes operators that are invariant under the Poincaré group (infrared operators). This property has been already noticed for the massless scalar two-dimensional field,[15] and appears naturally when the confining infrared singularities are controlled by a maximal Hilbert structure. In Sec. III, we turn our attention to the symmetries of the model; their treatment has unconventional features due to the indefiniteness of the theory. The equations of motion are invariant under the group $\mathscr{G}$ of local

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gauge transformations $\phi \to \phi + \alpha$, where α is a smooth real solution of the equation $\Box\alpha = 0$. The subgroup of global gauge transformations $\alpha = \text{const}$ is not broken in K and its generator is constructed using the infrared operators. Also, the scale transformations are implementable in the space K and, in fact, the translationally invariant operator, which was introduced as a new dynamical variable to account for the scale transformations of ϕ (Refs. 8 and 9) is here an intrinsic element of the theory and is exactly the infinitely delocalized limit of ϕ. In Sec. IV, we reconsider the problem of the quantization of the dipole field using the canonical formalism.

Finally, in Sec. V, we discuss the physical interpretation of the model. Our proposal is very different from those of Refs. 6, 7, 16, and 17. The authors of Ref. 6 obtain a Poincaré invariant Hilbert space with positive metric but they represent the field by a non-Hermitian operator and give up the relation between the Wightman functions and the scalar product in the physical space (from this point of view their solution has essentially changed the terms of the problem!). On the other hand, a rigid application of the requests of gauge invariance of the fields and Poincaré invariance of the physical space forces the authors of Ref. 7, 16, and 17 to conclude that the theory has a trivial content. On the contrary, we will show that the model may have a nontrivial physical meaning; we will prove that the severe singularities of the theory imply that the Poincaré group must be broken in every nontrivial physical space (mechanism of confinement); in particular, we will construct two positive quantizations of the dipole; in the first one, the time translations are broken while the space translations are an exact symmetry and the contrary happens in the second one. However, it is possible to define a vacuum sector that is the same for the two quantizations and with the property that the whole translation group is implementable on it.

II. THE HILBERT–KREIN STRUCTURE ASSOCIATED TO THE DIPOLE FIELD

A local and covariant quantization of the dipole field is characterized by a set of Wightman functions $\{\mathscr{W}_n\}$ satisfying the following axioms.

A. Temperedness

Here, $\mathscr{W}_n$ is a distribution belonging to $\mathscr{S}'(\mathbf{R}^{4n})$, the dual of the Schwartz space of the rapidly decreasing functions.[18]

B. Covariance

For any Poincaré transformation $\{a, \Lambda\}$ the n-point functions are invariant:

$$\mathscr{W}_n(\Lambda x_1 + a,...,\Lambda x_n + a) = \mathscr{W}_n(x_1,...,x_n). \tag{2.1}$$

C. Locality

If $x_i - x_{i+1} = \xi_i$ is spacelike, then

$$\mathscr{W}_n(x_1,...,x_i,x_{i+1},...,x_n) = \mathscr{W}_n(x_1,...,x_{i+1},x_i,...,x_n). \tag{2.2}$$

D. Weak spectral condition

The Fourier transforms $\tilde{W}(k_1,...,k_{n-1})$ of the distributions $W_n(\xi_1,...,\xi_{n-1}) = \mathscr{W}_n(x_1,...,x_n)$, have support contained in the cones

$$C_i^+ = \{(k_i)^\mu (k_i)_\mu \geqslant 0, (k_i)_0 \geqslant 0\}. \tag{2.3}$$

The Fourier transforms of test functions and distributions are defined by the following formulas:

$$\tilde{f}(k_1,...,k_n) = (2\pi)^{-2n} \int \exp(ik_1x_1 + \cdots + ik_nx_n) \times f(x_1,...,x_n)dx_1\cdots dx_n, \tag{2.4}$$

$$\tilde{T}(f) = T(\tilde{f}), \tag{2.5}$$

where kx is the Lorentz invariant product, $f \in \mathscr{S}(\mathbf{R}^{4n})$ and $T \in \mathscr{S}'(\mathbf{R}^4)$. These axioms and the equation of motion (1.1) lead us to the following two-point function:

$$\mathscr{W}_2(x_1,x_2) = W(\xi) = -(16\pi^2)^{-1} \ln(-\xi^2 + i\epsilon\xi_0). \tag{2.6}$$

We assume that the one-point function and all the truncated n-point functions vanish. As shown in Ref. 10 these Wightman functions define only a representation of the dipole field that is an operator-valued distribution on a linear space $\mathscr{D}$ (the local states): Indeed, one considers the Borchers algebra $\mathscr{B}$, which is the set of finite sequences $\mathbf{f} = (f_0,...,f_j,...)$ with $f_0 \in \mathbf{C}, f_j \in \mathscr{S}(\mathbf{R}^{4j})$; in $\mathscr{B}$, one defines the following inner product:

$$\langle \mathbf{f},\mathbf{g} \rangle = \sum_n \mathscr{W}_n(\mathbf{f}^* \times \mathbf{g})_n, \tag{2.7}$$

where $(\mathbf{f} \times \mathbf{g})_n = \Sigma_{k+1=n} f_k g_l$, $f^*(x_1,...,x_n) = \bar{f}(x_n,...,x_1)$ and the bar means complex conjugation.

Then, $\mathscr{D}$ is defined to be $\mathscr{B}/\mathscr{I}$; $\mathscr{I}$ is the Wightman ideal:

$$\mathscr{I} = \{\mathbf{f} \in \mathscr{B} : \langle \mathbf{f},\mathbf{g} \rangle = 0, \forall \mathbf{g} \in \mathscr{B}\} \tag{2.8}$$

(it is an ideal of $\mathscr{B}$ with respect to the product x). Elements of $\mathscr{D}$ are denoted by the symbol $[\mathbf{f}]$. By construction the inner product (2.7) is nondegenerate on $\mathscr{D}$. We may define the field operator on $\mathscr{D}$ as follows:

$$\phi(f)[\mathbf{g}] = [\mathbf{f} \times \mathbf{g}], \tag{2.9}$$

where a representative for $\mathbf{f}$ is $(0,f,0,...)$. It is clear that the vacuum vector Ψ_0, whose representative is $(1,0,...)$, is cyclic with respect to $\mathscr{F}$, the polynomial algebra generated by the fields $\phi(f)$. There is a linear representation of the Poincaré group on $\mathscr{D}$, defined by

$$U(a,\Lambda)[\mathbf{f}] = [\mathbf{f}_{\{a,\Lambda\}}], \tag{2.10}$$

where $f_{\{a,\Lambda\}}(x) = f(\Lambda^{-1}(x-a))$. The covariance of the Wightman functions implies that the operators $U(a,\Lambda)$ preserve the inner product (2.7) (η-unitary operators).

In the following, we will shortly denote by the same symbol f the test function entering in the field $\phi(f)$ and the

corresponding vector obtained by applying that field to the vacuum.

A supplement of information is now necessary if one wants to get a Hilbert space which represents the theory. The following condition[10] replaces the standard axiom of positivity.[11]

E. Hilbert space structure condition

There exists a set of Hilbert seminorms $\{p_n\}$, p_n defined on $\mathscr{S}(\mathbf{R}^{4n})$ and $\mathscr{S}$ continuous, such that

$$|\mathscr{W}_{n+m}(f_n^* \times g_m)| \leqslant p_n(f_n) p_m(g_m). \tag{2.11}$$

Without loss of generality we may assume in addition that these seminorms vanish on $\mathscr{I}$. Using standard methods, we may now complete $\mathscr{D}$ with respect to the topology induced by the seminorms $\{p_n\}$ and get a Hilbert space H. The more, we can extend the inner product (2.7) to the whole H and there exists a bounded and self-adjoint operator η such that[19]

$$\langle \Psi^1, \Psi_2 \rangle = (\Psi_1, \eta \Psi_2), \quad \forall \Psi_1, \Psi_2 \in H, \tag{2.12}$$

where $(\ ,\ )$ is the Hilbert scalar product in H, defined by the seminorms $\{p_n\}$. It is worth it to point out again that different choices of the seminorms give rise to different Hilbert spaces and whereas in the standard case the Wightman functions uniquely fix the closure of $\mathscr{D}$, in the indefinite metric case different closures are available corresponding to different topologies.

In our case, the factorization of the n-point functions (free-field theory) implies that a possible set of seminorms may be constructed using a single seminorm p defined on $\mathscr{S}(\mathbf{R}^4)$. We denote the inner product induced in $\mathscr{S}(\mathbf{R}^4)$ by the definition (2.7) by the same symbol $\langle\ ,\ \rangle$. It is possible to choose a $\chi \in \mathscr{S}(\mathbf{R}^4)$ such that $\tilde{\chi}(0) = 1$ and $\langle \chi, \chi \rangle = 0$ (Ref. 7). Then one has that[20]

$$\langle f,g \rangle = \frac{1}{2}\pi \int \{(1-D)[\bar{\tilde{f}}_0(k)\tilde{g}_0(k) + \bar{\tilde{f}}(0)\tilde{\chi}(k) g_0(k) + \tilde{g}(0)\bar{\tilde{f}}_0(k)\tilde{\chi}(k)]\}|_{c_+} \omega^{-3} d^3\mathbf{k}, \tag{2.13}$$

with $f_0(k) = f(k) - \tilde{f}(0)\chi(k)$, $D\tilde{f}(k) = k_0 \partial/\partial k_0 \tilde{f}(k)$, and $\omega^2 = k_1^2 + k_2^2 + k_3^2$. We now define a Hilbert product in $\mathscr{S}(\mathbf{R}^4)$ as follows:

$$(f,g) = \frac{1}{2}\pi \int [\bar{F}_1(\mathbf{k}) G_1(\mathbf{k}) + \bar{F}_2(\mathbf{k}) G_2(\mathbf{k})] \omega^{-3} d^3\mathbf{k} + \langle f,\chi \rangle \langle \chi, g \rangle + \bar{\tilde{f}}(0)\tilde{g}(0), \tag{2.14}$$

with

$$F_1(\mathbf{k}) = [(1-D)\tilde{f}_0(k)]|_{c_+} \quad \text{and} \quad F_2(\mathbf{k}) = [D\tilde{f}_0(\mathbf{k})]|_{c_+}. \tag{2.15}$$

It is easy to see that $|\langle f,g \rangle| \leqslant \|f\| \, \|g\|$, with $\|f\|^2 = (f,f)$. Now we have that the vectors

$$\Psi^n_{f_1 \cdots f_n} = (n!)^{-1/2} : \phi(f_1) \cdots \phi(f_n) : \Psi_0 \tag{2.16}$$

generate $\mathscr{D}$. The symbol : : denotes the Wick-ordered product defined in terms of Wightman functions.[21] It follows that

$$\langle \Psi^n_{f_1,\ldots,f_n}, \Psi^m_{g_1,\ldots,g_m} \rangle = (n!)^{-1} \delta_{n,m} \sum_\pi \langle f_1, g_{i_1} \rangle \cdots \langle f_n, g_{i_n} \rangle, \tag{2.17}$$

where Σ_π denotes the sum over all the permutations. We may now define a Hilbert product in $\mathscr{D}$ simply by

$$(\Psi^n_{f_1,\ldots,f_n}, \Psi^m_{g_1,\ldots,g_m}) = (n!)^{-1} \delta_{n,m} \sum_\pi (f_1, g_{i_1}) \cdots (f_n, g_{i_n}). \tag{2.18}$$

Denoting by K the Hilbert completion of $\mathscr{D}$ with respect to the topology induced by the (2.18), it follows that

$$K = \oplus_n K^{(n)}, \quad K^{(n)} = \otimes_s^n K^{(1)}, \tag{2.19}$$

where $K^{(1)}$ is the Hilbert completion of $\mathscr{S}(\mathbf{R}^4)$ and $\otimes_s$ denotes the symmetric tensor product. Therefore, the study of $K^{(1)}$ completely fixes the Hilbert space of the theory. The main result of this section consists in the proof that K is a Krein space. To prove this, we need to study in advance the space $H^{(1)}$, which is the completion of the space

$$\mathscr{S}_0(\mathbf{R}^4) = \{f \in \mathscr{S}(\mathbf{R}^4) : \tilde{f}(0) = 0\} \tag{2.20}$$

with respect to the Hilbert topology induced by the scalar product

$$[f,g] = \frac{1}{2}\pi \int [\bar{F}_1(\mathbf{k}) G_1(\mathbf{k}) + \bar{F}_2(\mathbf{k}) G_2(\mathbf{k})] \omega^{-3} d^3\mathbf{k}. \tag{2.21}$$

Lemma 2.1: It is possible to extend the product (2.13) to the whole $H^{(1)}$ and there exists a bounded and self-adjoint operator η_0 such that

$$\langle f,g \rangle = [f, \eta_0 g], \quad \forall f,g \in H^{(1)}, \tag{2.22}$$

and besides

$$(\eta_0)^2 = 1; \tag{2.23}$$

i.e., $H^{(1)}$ is a Krein space.

Proof: The first part of the lemma follows from standard theorems of functional analysis.[19] We need only to show the (2.23). To this end, we consider the space $\mathscr{S}_0(R^4) \otimes C^2$ endowed with the products

$$\{F,G\}_\pm = \frac{1}{2}\pi \int [\bar{\tilde{f}}_1(k)\tilde{g}_1(k) \pm \bar{\tilde{f}}_2(k)\tilde{g}_2(k)]|_{c_+} \omega^{-3} d^3\mathbf{k}, \tag{2.24}$$

and a map U: $\mathscr{S}_0(R^4) \to \mathscr{S}_0(R^4) \otimes C^2$ defined by

$$U\tilde{f} = \begin{bmatrix} (1-D)\tilde{f} \\ D\tilde{f} \end{bmatrix}. \tag{2.25}$$

It is obvious that we may extend the operator U to an operator $\bar{U}$ defined on $H^{(1)}$ with values in the Hilbert completion of $\mathrm{ran}(U)$ with respect to the topology induced by the product $\{\ ,\ \}_+$, which we denote by $\overline{R(U)}$. The operator $\bar{U}$ has the following properties:

$$\{\bar{U}f, \bar{U}g\}_+ = [f,g], \quad \{\bar{U}f, \bar{U}g\}_- = \langle f,g \rangle, \tag{2.26}$$

$\forall f,g \in H^{(1)}$. Besides, one has that

$$\{\bar{U}f, \bar{U}g\}_- = \{\bar{U}f, \sigma_3 \bar{U}g\}_+ \tag{2.27}$$

with $(\sigma_3)_{i,j} = \delta_{i,j}(-1)^{i+1}$. Therefore, it follows that

$$\{\overline{U}f,\overline{U}\eta_0 g\}_+ = [f,\eta_0 g] = \langle f,g\rangle = \{\overline{U}f,\overline{U}g\}_- = \{\overline{U}f,\sigma_3\overline{U}g\}_+, \tag{2.28}$$

$\forall f,g\in H^{(1)}$. It is now possible to show that σ_3 maps $\overline{R(U)}$ into itself; this implies that we may apply Eq. (2.28) twice and obtain that

$$[f,(\eta_0)^2 g] = \{\overline{U}f,(\sigma_3)^2\overline{U}g\}_+ = \{\overline{U}f,\overline{U}g\}_+ = [f,g]. \tag{2.29}$$

This relation is valid $\forall f,g\in H^{(1)}$ and this implies (2.23).

The fact that D is a differential operator nontangential to the future cone C_+ implies that $\overline{R(U)}$ is isomorphic to the Hilbert space $L^2(C_+ - \{0\},\omega^{-3}\,d^3\mathbf{k})\otimes\mathbf{C}^2$, which we briefly denote $L^2\otimes\mathbf{C}^2$. The use of the operator $\overline{U}$ makes possible the proof of the following.

Corollary 2.2: $H^{(1)}$ is isomorphic to $L^2\otimes\mathbf{C}^2$, which is the space of two complex component functions, defined on $\{C_+ - \{0\}\}$, square integrable with respect to the measure $\omega^{-3}\,d^3\mathbf{k}$.

We are now in a position to state and prove the main theorem of this section.

Theorem 2.3: It is possible to extend the inner product (2.13) to the whole $K^{(1)}$ and there exists a bounded and self-adjoint operator $\eta^{(1)}$ such that $\forall f,g\in K^{(1)}$, it happens that

$$\langle f,g\rangle = (f,\eta^{(1)}g), \tag{2.30}$$

$$(\eta^{(1)})^2 = 1. \tag{2.31}$$

Proof: As in precedence we need only to show Eq. (2.31). Let us define from $K^{(1)}$ the following functional:

$$X(f) = \langle\chi,f\rangle. \tag{2.32}$$

This functional is continuous because $|X(f)|\leqslant\|f\|$; actually it is possible to show that its norm is exactly one: Indeed, if we take the sequence of elements of $\mathscr{S}_0(\mathbf{R}^4)$ defined by

$$\tilde{f}_n^{\chi}(k) = \vartheta_n(\omega)\tilde{\chi}(k), \tag{2.33}$$

with $\vartheta(t)$ an infinitely differentiable nondecreasing real function, which is zero for $t\leqslant 0$ and is one for $t\geqslant 1$, and $\vartheta_n(t) = \vartheta(nt)$, we find that

$$|X(f_n)|/\|f_n\| \underset{n\to\infty}{\to} 1. \tag{2.34}$$

The Riesz lemma implies that there exists a vector $v^+\in K^{(1)}$ such that $(v^+,v^+) = 1$ and $\forall f\in K^{(1)}$

$$\langle\chi,f\rangle = (v^+,f). \tag{2.35}$$

It is not difficult to show that the sequence

$$v_n^+ = (\langle\chi,f_n^{\chi}\rangle)^{-1} f_n^{\chi} \tag{2.36}$$

converges to v^+ in $K^{(1)}$. We may think to $K^{(1)}$ as decomposed into orthogonal subspaces

$$K^{(1)} = K_0^{(1)}\oplus V^+\oplus X \tag{2.37}$$

where V^+ and X are the one-dimensional subspaces generated by v^+ and χ and

$$K_0^{(1)} = \{f\in K^{(1)}:(\chi,f) = (v^+,f) = 0\}. \tag{2.38}$$

It follows from the formulas (2.13, 14, 38) and the Corollary 2.2 that $K_0^{(1)}$ is isomorphic to $L^2\otimes\mathbf{C}^2$.

Now, we want to compute explicitly the action of the metric operator $\eta^{(1)}$ on the subspace $V^+\oplus X$. We have that for any $f\in K^{(1)}$

$$(v^+,f) = \langle\chi,f\rangle = (\eta^{(1)}\chi,f), \tag{2.39}$$

and this implies $\eta^{(1)}\chi = v^+$. Now, let $f\in\mathscr{S}(\mathbf{R}^4)$. We have that

$$(\chi,f) = \tilde{f}(0), \tag{2.40}$$

$$\langle v^+,f\rangle = \lim\langle v_n^+,f\rangle = \tilde{f}(0) = (\eta^{(1)}v^+,f). \tag{2.41}$$

The density of $\mathscr{S}(\mathbf{R}^4)$ finally implies that $\eta^{(1)}v^+ = \chi$. We may write

$$f = Pf + (v^+,f)v^+ + (\chi,f)\chi,\quad \forall f\in K^{(1)}, \tag{2.42}$$

where P is the projector on $K_0^{(1)}$. From Eq. (2.42), it follows that

$$\langle f,g\rangle = (f,P\eta^{(1)}Pg) + (f,v^+)(\chi,g) + (f,\chi)(v^+,g). \tag{2.43}$$

Theorem 2.1 and the decomposition (2.37) imply that $P\eta^{(1)}P = P\eta_0^{(1)}P$. Defining by $P_\pm$ the projectors on the vectors $2^{-1/2}(v^+\pm\chi)$, we obtain

$$\langle f,g\rangle = (f,\eta^{(1)}g) = (f,\{P\eta_0^{(1)}P + P_+ - P_-\}g) \tag{2.44}$$

and, therefore,

$$\eta^{(1)} = P\eta_0^{(1)}P + P_+ - P_-. \tag{2.45}$$

Equation (2.45) finally implies that $(\eta^{(1)})^2 = 1$.

Corollary 2.4: $K^{(1)}$ is isomorphic to $(L^2\otimes\mathbf{C}^2)\oplus V^+\oplus X$.

Corollary 2.5: K is a Krein space.

The implementers of the Poincaré group are η-unitary but unbounded, and therefore they are defined only on a dense set. We remark that the sequence (2.36) converges pointwise to zero; this means that the vector v^+ is not a function and it describes a Poincaré invariant state (infrared state); indeed it is easy to prove that v^+ belongs to the domain of the operators $U(a,\Lambda)$; then, $\forall f\in\mathscr{S}(\mathbf{R}^4)$, we have

$$\langle\{U(a,\Lambda)v^+ - v^+\},f\rangle = \langle v^+,f_{\{a,\Lambda\}}\rangle - \langle v^+,f\rangle = \tilde{f}(0) - \tilde{f}(0) = 0. \tag{2.46}$$

The density of $\mathscr{S}(\mathbf{R}^4)$ and the nondegeneracy of the inner product (2.13) implies that

$$U(a,\Lambda)v^+ = v^+. \tag{2.47}$$

However, the vector v^+ has zero η norm. This implies that the vacuum vector is essentially unique;[10] i.e., there is no positive subspace of translationally invariant vectors, whose dimension is greater than one. We may represent the field operator in K by the following formula:

$$(\phi(f)\Psi)^{(n)} = (n+1)^{-1/2}\langle\bar{f},\Psi^{(n+1)}\rangle(k_1,\ldots,k_n) + (n)^{-1/2}\times\sum_{j=1}^{n}\tilde{f}(k_j)\Psi^{(n-1)}(k_1,\ldots,\not{k}_j,\ldots,k_n) \tag{2.48}$$

where the f appearing at the r.h.s. has to be regarded as an element of $K^{(1)}$, $\Psi^{(m+1)} = \Psi^{(m+1)}(k,k_1,\ldots,k_n)$ and k is the "integrated" variable. This formula also gives explicit expressions for the positive and negative frequencies parts of

the field operator. Note that with our conventions on the Fourier transforms of distributions, positive frequencies correspond to "creation" operators. Also the covariance of the field follows easily by (2.48). When the smearing function f is real, the operator $\phi(f)$ is essentially self-adjoint with respect to the indefinite product (η self-adjoint). The following estimate may be proven using the representation (2.48), exactly as in the ordinary case:[19]

$$\|\phi(f)\Psi^{(m)}\| \leqslant (m+1)^{1/2}(\|f^+\| + \|f^-\|), \quad (2.49)$$

with $\tilde{f}^{\pm}(k) = \tilde{f}(\pm k)$. We may now define another seminorm on $\mathscr{S}(\mathbf{R}^4)$ by

$$q(f)^2 = \|f^+\|^2 + \|f^-\|^2. \quad (2.50)$$

The completion of $\mathscr{S}(\mathbf{R}^4)$ with respect to the topology induced by the seminorm q gives, exactly as before, the space

$$\begin{aligned}&(L^2(C_+ - \{0\}, \omega^{-3}\, d^3\mathbf{k}) \otimes \mathbf{C}^2)\\ &\quad \oplus (L^2(C_- - \{0\}, \omega^{-3}\, d^3\mathbf{k}) \otimes \mathbf{C}^2)\\ &\quad \oplus V^+ \oplus V^- \oplus X, \end{aligned} \quad (2.51)$$

where v^- is the one-dimensional subspace generated by the vector $v^- = \lim v_n^-$. By (2.49), we see that the sequence

$$\{\Psi_{f_{n_1},\ldots,f_{n_k}}\} = \{:\phi(f_{n_1},\ldots,f_{n_k}):\Psi_0\} \quad (2.52)$$

converges in K if each of the $\{f_n\}$ converges in the space (2.51). It follows that the local field algebra $\mathscr{F}$ has an extension $\mathscr{F}_{\text{ext}}$ which contains the fields $\phi(f)$, with f belonging to the space (2.51). In particular, $\mathscr{F}_{\text{ext}}$ encloses the infrared field operators $\phi(v^+)$ and $\phi(v^-)$, which are invariant under the Poincaré group.

We stress again that the existence of the infrared state and operators is a consequence of the fact that K is a maximal space associated with the given Wightman functions; this feature is not shared by non-Krein realizations of the theory.

III. SYMMETRIES

The construction of the Hilbert–Krein space of the theory allows a correct discussion of the questions concerning the symmetries of the model. We have already discussed the Poincaré symmetry and we will again turn our attention to it when we treat the physical interpretation of the model. Another very important symmetry of this model is the gauge symmetry; in fact, one sees immediately that the equation of motion (1.1) is invariant under the following gauge transformations of the second kind (local gauge transformations):

$$\phi \to \phi + \alpha, \quad (3.1)$$

where α is a real smooth solution of the equation $\Box\alpha = 0$. There is an important class of solutions of this equation, given by the equation $\alpha(x) = \lambda = \text{const}$. These solutions are called gauge transformations of the first kind (global transformations); they define the following automorphism of the field algebra:

$$\gamma^\lambda : \phi(x) \to \phi(x) + \lambda. \quad (3.2)$$

It is instructive to consider this case to see how different the treatment of symmetries is in the indefinite metric case with respect to the standard case. Consider the following local charge:

$$Q_R = \int \partial_0 \Box\phi(x) f_R(\mathbf{x}) \alpha_d(x_0)\, d^4x, \quad (3.3)$$

where $f(x)$ is an indefinitely differentiable function such that $f(\mathbf{x}) = 1$, if $|\mathbf{x}| \leqslant 1$, and $f(x) = 0$, if $|\mathbf{x}| \geqslant 2$, and $\alpha_d(x_0)$ is an infinitely differentiable function of compact support such that

$$\int \alpha_d(x_0)\, dx_0 = 1, \quad \lim_{d\to 0} \alpha_d(x_0) = \delta(x_0). \quad (3.4)$$

One has

$$\begin{aligned}\frac{d}{d\lambda}\gamma^\lambda(\phi(f))|_{\lambda=0} &= i \lim_{R\to\infty} [Q_R, \phi(f)]\\ &= (2\pi)^2 \tilde{f}(0) = \int f(x)\, d^4x. \end{aligned} \quad (3.5)$$

Theorem 4.1: The automorphism γ^λ is implementated in the Krein space K by the operator $\Gamma^\lambda = \exp 2\pi^2 i\lambda Q$, with $Q = (2\pi^2)^{-1} w - \lim Q_R$.

Proof: Define

$$Q = i[\phi(v^+) - \phi(v^-)]. \quad (3.6)$$

It is easy to see that Q_R converges to $(2\pi^2)Q$ as a bilinear form on $\mathscr{D} \times \mathscr{D}$. Besides, one has the following uniform majorization

$$\|\partial_0 \Box\phi(f_R \alpha_d)\Psi\| \leqslant \text{const}. \quad (3.7)$$

This implies that Q_R is weakly convergent to $2\pi^2 Q$. Now we have $\mathscr{D}$ as a set of analytic vectors for Q and therefore we may exponentiate it and obtain

$$\Gamma^\lambda = \exp 2\pi^2 i Q. \quad (3.8)$$

The fact that Γ^λ actually implements the symmetry γ^λ is now evident.

Thus the global gauge symmetry is unbroken in the Krein space (i.e., there exists a one-parameter group of η-unitary operators implementing the global gauge transformations). We remark that this symmetry would have been broken if we had used a non-Krein topology (see the analogous mechanism in Ref. 15). Here emerges a feature that is not shared by conventional theories: The symmetry is implementable but the vacuum is not invariant under the action of the implementers Γ^λ. It is, however, essentially invariant: Indeed the extra term is a translationally invariant null vector. Another very interesting symmetry of the theory is given by the scale transformations $x \to sx$. These transformations act on the two-point function by adding the constant $-(8\pi^2)^{-1} \ln s$. Let us define the following automorphism of $\mathscr{F}_{\text{ext}}$:

$$\alpha_s : \phi(f) \to \phi(f_s) + \tfrac{1}{4}\pi^2 \ln s \tilde{f}(0)\phi(v), \quad (3.9)$$

with

$$f_s(x) = s^{-4} f(x/s) \text{ and } \phi(v) = \phi(v^+) + \phi(v^-). \quad (3.10)$$

Theorem 4.2: The automorphism α_s is implemented in the Krein space K by the operators $U(s)$ which are η-unitary and leave the vacuum invariant.

Proof: It is easy to verify that

$$\langle \Psi_0, \alpha_s(\phi(f))\alpha_s(\phi(g))\Psi_0\rangle = \langle \Psi_0, \phi(f)\phi(g)\Psi_0\rangle. \quad (3.11)$$

The action of $U(s)$ is determined by its definition on the one-particle space:

$$U(s)\Psi_f = \Psi_{f_s} + \tfrac{1}{4}\pi^2\tilde{f}(0)\log s v^+ \tag{3.12}$$

and because of the invariance of the Wightman functions one has

$$U(s)\Psi_0 = \Psi_0. \tag{3.13}$$

We see here that the translationally invariant operator that has been introduced in literature as a new dynamical variable to account for the scale transformations of ϕ in the context of conformally invariant models,[8,9] is exactly $\phi(v)$, the infinitely delocalized limit of ϕ; it is therefore an intrinsic content of the model in the Krein space approach.

IV. CANONICAL QUANTIZATION

In this section, we want to reconsider the problem of the quantization of the dipole field from an algebraic point of view. To this end, we consider an abstract (i.e., not realized) operator-valued distribution ϕ, obeying to the equation $\Box\phi = 0$ and to the commutation rules

$$[\phi(x),\phi(y)] = -(i/8\pi)\epsilon(\xi_0)\vartheta(\xi^2), \tag{4.1}$$

where $\vartheta(t)$ is the step function and $\epsilon(t) = \vartheta(t) - \vartheta(-t)$; the commutator (4.1) follows immediately by the two-point function (2.6). To avoid ambiguities, we restrict test functions to those of $\mathscr{S}(\mathbf{R}^4)$. It is then possible to introduce in a standard way[11] the splitting of the field ϕ into positive and negative frequency parts $\phi = \phi^+ + \phi^-$. General properties of hyperbolic equations[22] allow us to extend the possible test functions to distributions of the form $f_t(x) = \delta(x_0 - t)f(\mathbf{x})$ with $f \in \mathscr{S}_0(\mathbf{R}^3)$. The commutator (4.1) then implies that the only nonzero fixed time commutators are the following:

$$\begin{aligned}[\phi(t,\mathbf{x}),\partial_0\Box\phi(t,\mathbf{y})] &= [\Box\phi(t,\mathbf{x}),\partial_0\phi(t,\mathbf{y})] \\ &= i\delta^3(\mathbf{x}-\mathbf{y}).\end{aligned} \tag{4.2}$$

The commutators (4.2) are exactly those that one imposes in the canonical quantization of a system of two fields with Lagrangian[4]

$$\mathscr{L} = \partial^\mu\phi\partial_\mu\Lambda + \tfrac{1}{2}\Lambda^2. \tag{4.3}$$

Actually Λ is not independent on ϕ: Indeed the equations of motion that follow from (4.3) are

$$\Box\phi = \Lambda, \quad \Box\Lambda = 0 \tag{4.4}$$

(which together imply $\Box^2\phi = 0$). We consider then the star algebra generated by the fields $\phi^{(\pm)},\partial_0\phi^{(\pm)},\Lambda^{(\pm)},\partial_0\Lambda^{(\pm)}$, taken at $t = 0$ [i.e., smeared with test functions of the form $\delta(x_0)f(\mathbf{x})$]. Clearly, not all of these fields are algebraically independent: Indeed they are linked by the four relations given by conjugation and by the two commutators (4.3). Taking these relations into account, we are led to the fields

$$\begin{aligned}\psi_1(0,\mathbf{x}) &= (-\Delta)^{3/4}\phi(0,\mathbf{x}) + i(-\Delta)^{1/4}\partial_0\phi(0,\mathbf{x}) \\ &\quad + (i/2)(-\Delta)^{-3/4}\partial_0\Lambda(0,\mathbf{x}),\end{aligned} \tag{4.5}$$

$$\begin{aligned}\psi_2(0,\mathbf{x}) &= (-\Delta)^{3/4}\phi(0,\mathbf{x}) + i(-\Delta)^{1/4}\partial_0\phi(0,\mathbf{x}) \\ &\quad - \tfrac{1}{2}(-\Delta)^{-1/4}\Lambda(0,\mathbf{x}).\end{aligned} \tag{4.6}$$

By construction, these fields contain only negative frequencies (and, therefore, when conjugated contain only positive frequencies); we may obtain two pairs of creation and annihilation operators simply by Fourier transform:

$$a_i(\mathbf{k}) = (2\pi)^{-3/2}\int \exp(i\mathbf{kx})\psi_i(0,\mathbf{x})d^3\mathbf{x}, \tag{4.7}$$

$$a_i^\dagger(\mathbf{k}) = (2\pi)^{-3/2}\int \exp(-i\mathbf{kx})\psi_i^\dagger(0,\mathbf{x})d^3\mathbf{x}. \tag{4.8}$$

These operators satisfy to the following (pseudo) canonical commutation relations:

$$[a_1(\mathbf{q}),a_1^\dagger(\mathbf{k})] = \delta^3(\mathbf{q}-\mathbf{k}), \tag{4.9}$$

$$[a_2(\mathbf{q}),a_2^\dagger(\mathbf{k})] = -\delta^3(\mathbf{q}-\mathbf{k}). \tag{4.10}$$

The remaining commutators are zero. We remark that the minus sign at the r.h.s. is an unavoidable consequence of the relation between the spectral condition and the splitting of the field operator into positive and negative frequencies. Obviously, one may take a combination of these operators to obtain the canonical commutation relatons (C.C.R.) in the usual form (without the minus sign), but the so obtained operators are no longer related to the positive and negative frequency pairs of the field (for instance, this relation is lost in the treatment of the dipole given in Ref. 4). The field equation determines the following time evolution of the a's:

$$\tau_t(a_1(\mathbf{k})) = \exp(-i\omega t)[(1+i\omega t)a_1(\mathbf{k}) - i\omega t a_2(\mathbf{k})], \tag{4.11}$$

$$\tau_t(a_2(\mathbf{k})) = \exp(-i\omega t)[i\omega t a_1(\mathbf{k}) + (1-i\omega t)a_2(\mathbf{k})]. \tag{4.12}$$

Therefore, the time evolution mixes a_1 with a_2; however, it is not a Bogoliubov transformation because it does not mix creators and annihilators. Using the previous formulas, one may obtain the following representation of the field:

$$\begin{aligned}\phi(t,\mathbf{x}) &= (2\pi)^{-3/2}\int \exp(i\omega t - i\mathbf{kx})[(1-i\omega t)a_1^\dagger(\mathbf{k}) \\ &\quad + i\omega t\, a_2^\dagger(\mathbf{k})](2\omega^{3/2})^{-1}d^3\mathbf{k} \\ &\quad + (2\pi)^{-3/2}\int \exp(-i\omega t + i\mathbf{kx}) \\ &\quad \times[(1+i\omega t)a_1(\mathbf{k}) - i\omega t\, a_2(\mathbf{k})](2\omega^{3/2})^{-1}d^3\mathbf{k}.\end{aligned} \tag{4.13}$$

The commutation relations (4.9) and (4.10) also imply that the Fock space in which the whole canonical algebra is represented must have an indefinite metric. The Fock vacuum is defined by the following conditions:

$$a_1(\mathbf{k})\Omega = a_2(\mathbf{k})\Omega = 0. \tag{4.14}$$

The usual methods of Lagrangian field theory lead us to the following four momentum:

$$\begin{aligned}H &= \int \omega[a_2^\dagger(\mathbf{k})(a_1(\mathbf{k}) - a_2(\mathbf{k})) \\ &\quad + (a_1^\dagger(\mathbf{k}) - a_2^\dagger(\mathbf{k}))a_2(\mathbf{k})]d^3\mathbf{k}\end{aligned} \tag{4.15}$$

$$P^i = \int k^i[a_1^\dagger(\mathbf{k})a_1(\mathbf{k}) - a_2^\dagger(\mathbf{k})a_2(\mathbf{k})]d^3\mathbf{k}. \tag{4.16}$$

The Hamiltonian given in the (4.14) does indeed generate the time evolution τ_t; in fact, one has

$$\frac{d}{dt}\tau_t(a_i(\mathbf{k}))|_{t=0} = i[H,a_i(\mathbf{k})]. \tag{4.17}$$

Therefore, the time evolution is implementable in the (indefinite metric) Fock space of the model. We will return again to this canonical formalism in the next chapter when we will discuss the physical interpretation of the model.

V. THE PHYSICAL INTERPRETATION

It is necessary at this point to identify some subspace K' of the Krein space K by means of which constructing the physical space of the theory. Here K' must satisfy at least the two following requirements: The vacuum vector must belong to K' (i.e., the vacuum is a physical state); and K' must be semidefinite (i.e., $\langle\Psi,\Psi\rangle \geqslant 0$, $\forall\Psi\in K'$) for the probabilistic interpretation of the theory. It is usual to define the space K' using an operatorial supplementary condition, as in the Gupta–Bleuler or B.R.S.T. quantization. Then, defining

$$K'' = \{\Psi\in K' : \langle\Psi,\Psi\rangle = 0\}, \tag{5.1}$$

we obtain as a candidate for the physical space of the theory the following Hilbert space:

$$K_{\text{phys}} = \overline{(K'/K'')}, \tag{5.2}$$

where the completion is taken with respect to the Hilbert topology induced by the scalar product $\langle\ ,\ \rangle$. Before performing the explicit construction of some possible physical spaces, we state and prove the following important no-go theorem.

Theorem 5.1: Every semidefinite subspace of $\mathscr{D}$, invariant under space-time translations is a null subspace of $\mathscr{D}$.

Proof: It is clear that it is enough to show this result at the one particle level and, therefore, we consider a positive semidefinite subspace of $\mathscr{S}(\mathbf{R}^4)$ which contains a certain function f and all of its translated f_a; Eq. (2.10) implies that $\tilde{f}_a(k) = \exp(ika)\tilde{f}(k)$. Call this space $\mathscr{T}_f$. We use at first the invariance of $\mathscr{T}_f$ under time translations. Let $a = (t,\mathbf{0})$ and define

$$T_1(t) = \langle f - f_t, f - f_t\rangle. \tag{5.3}$$

By hypothesis, $T_1(t)\geqslant 0$ and it is obvious that $T_1(0) = 0$. Therefore, the point $t = 0$ must be a minimum for $T_1(t)$, and this implies that

$$\frac{d^2}{dt^2}T_1(t)|_{t=0}$$

$$= -\pi\int [(1+D)|\tilde{f}(k)|^2]|_{C_+}\,\omega^{-1}\,d^3\mathbf{k}\geqslant 0. \tag{5.4}$$

The same argument may be applied to the function

$$T_n(t) = \left\langle \sum_{j=0}\binom{n}{j}(-1)^j f_{jt}, \sum_{j=0}\binom{n}{j}(-1)^j f_{jt}\right\rangle. \tag{5.5}$$

By induction one has

$$\frac{d^m}{dt^m}T_n(t)|_{t=0} = 0, \quad m\leqslant 2n-1. \tag{5.6}$$

The fact that $t = 0$ must be a minimum for $T_n(t)$ now gives the condition

$$\int \omega^{2n-3}[(1-2n-D)|\tilde{f}(k)|^2]|_{C_+}\,d^3\mathbf{k}\geqslant 0. \tag{5.7}$$

Now we exploit the invariance of $\mathscr{T}_f$ under space translations. To illustrate the method let us suppose at first that $f\in\mathscr{S}_0(\mathbf{R}^4)$. The non-negativity of $\mathscr{T}_f$ implies that

$$\langle f,f\rangle = \frac{1}{2}\pi\int [(1-D)|\tilde{f}(k)|^2]|_{C_+}\,\omega^{-3}\,d^3\mathbf{k}\geqslant 0. \tag{5.8}$$

The invariance of $\mathscr{T}_f$ under space translations implies that, actually, it must be

$$[(1-D)|\tilde{f}(k)|]|_{C_+}\geqslant 0 \tag{5.9}$$

pointwise. Indeed, let us define

$$\tilde{F}_{\epsilon,N}(k) = \left(\frac{\epsilon}{N}\right)^{3/2}\sum_{n_1,n_2,n_3=-N}^{N}\exp(i\mathbf{q}n\epsilon)\tilde{f}_{n\epsilon}(k), \tag{5.10}$$

with $n\epsilon = (0,n_1\epsilon,n_2\epsilon,n_3\epsilon)$ and $\epsilon > 0$. When ϵ and N stay finite, $F_{\epsilon,N}$ belongs to $\mathscr{T}_f$ and, by hypothesis,

$$\langle F_{\epsilon,N},F_{\epsilon,N}\rangle$$
$$= \frac{1}{2}\pi\left(\frac{\epsilon}{n}\right)^3\sum_{\mathbf{n},\mathbf{m}=-N}^{N}\int\exp[i(\mathbf{k}-\mathbf{q})(\mathbf{n}-\mathbf{m})\epsilon]$$
$$\times(1-D)|\tilde{f}(k)|^2|_{C_+}\,\omega^{-3}\,d^3\mathbf{k}\geqslant 0. \tag{5.11}$$

By choosing $\epsilon = N^{-1/2}$ and taking the limit of the last expression for $N\to\infty$, we obtain (5.8). Repeating now the steps that led us to the formula (5.7), we conclude that it must be

$$\{(1-2n-D)|\tilde{f}(k)|^2\}|_{C_+}\geqslant 0, \quad \forall n\geqslant 1, \tag{5.12}$$

where it is no more necessary to suppose that $f\in\mathscr{S}_0(\mathbf{R}^4)$. It is now evident that the system of inequalities (5.12) may be verified if and only if

$$\tilde{f}(k)|_{C_+} = 0. \tag{5.13}$$

Therefore, $\mathscr{T}_f$ is contained in the linear space

$$\mathscr{N} = \{f\in\mathscr{S}(\mathbf{R}^4) : \tilde{f}(k)|_{C_+}\}, \tag{5.14}$$

which is a null subspace of $\mathscr{S}(\mathbf{R}^4)$ invariant under the translations group. Therefore, $\mathscr{T}_f$ is a null subspace of $\mathscr{S}(\mathbf{R}^4)$.

Corollary 5.2: Every semidefinite (actually null) translationally invariant subspace of $\mathscr{S}(\mathbf{R}^4)$ is contained in $\mathscr{N}$.

Thus, according to Corollary (5.2), there is no hope of obtaining a nontrivial physical space that be Poincaré invariant: Indeed, the condition (5.13) leads to a physical space that contains only the vacuum vector.[7,16,17] This fact does not mean that the content of the theory is trivial; it means only that we must construct a physical space in which the Poincaré symmetry is broken. This should not come as a surprise: Indeed, already in QED_4 the construction of the physical charged sectors requires the breaking of the Lorentz group.[23] Besides, confinement of charged massless particles in QED_4 and of charged massive particles in QED_3 is a consequence of the breaking of the translation group in the physical space.[24] Also, in the present case, the infrared singularities are of the confining type, and lead to the breaking of the translation group in the physical space (*mechanism of confinement*). Let us see the concrete construction of some possible physical spaces: Consider a complex valued infinitely differentiable function $z = z(k)$, such that

$$\text{Re}\,z(k) = \mu < 1/2, \quad |\text{Im}\,z(k)| < \text{const}|k|. \tag{5.15}$$

Each $z(k)$ that satisfies the previous conditions labels a possible physical space $K_{z,\mathrm{phys}}$. Indeed, following the procedure briefly illustrated at the beginning of this section, we may define the one particle space $K_z^{(1)}$ as the Krein closure of the dense set

$$\mathscr{D}_z^{(1)} = \{ f \in \mathscr{S}_0(\mathbf{R}^4) : (D - z(k))\tilde{f}(k)|_{C_+} \}. \tag{5.16}$$

Here, K_z' may be obtained as the symmetric Fock space over $K_z^{(1)}$, and the physical space $K_{z,\mathrm{phys}}$ is given by K_z'/K_z''. It is possible to see that K_z' is a maximal non-negative subspace of K (i.e., it is not properly contained in any other non-negative subspace of K). Note that the set (5.16) is not stable under the translation group; indeed one has

$$U(a)\mathscr{D}_z^{(1)} = \mathscr{D}_{z + ik_0 a_0}^{(1)}. \tag{5.17}$$

Equation (5.17) implies that K_z' is not stable under time translations while its stable under space translations; in particular the time translations map a dense set of a maximal non-negative subspace of K onto a dense set of another maximal non-negative subspace of K and therefore define orbits (of maximal non-negative subspaces of K).

The same happens for the Lorentz boosts, while purely spatial rotations leave each K_z' invariant.

To get a closer insight into the structure of these spaces we now study in some detail the case $z = 0$. We have

$$K_{z=0}^{(1)} = L^2(C_+ - \{0\}, \omega^{-3}\, d^3k) \oplus V^+, \tag{5.18}$$

$$K_{z=0}^{(1)\prime\prime} = V^+; \tag{5.19}$$

$$K_{z=0,\mathrm{phys}}^{(1)} = L^2(C_+ - \{0\}, \omega^{-3}\, d^3k). \tag{5.20}$$

The total physical space $K_{z=0,\mathrm{phys}}$ may be obtained by the usual Fock procedure. The fact that $K_{z=0}'$ is maximal semidefinite may be understood by looking at (5.18). Equation (2.48) implies that the vectors of $K_{z=0}'$ may be characterized by the following Gupta–Bleuler condition:

$$\phi^-(f)\Psi = 0, \quad \forall f \in \mathscr{S}_0(\mathbf{R}^4) \text{ such that } (1 - D)\tilde{f}(-k)|_{C_+} = 0,$$
$$\phi(v^-)\Psi = 0. \tag{5.21}$$

The next interesting question concerns the definition of the fields on the physical space. We distinguish here two notions of "quotientability" that are similar to those notions of gauge invariance introduced in Ref. 25. Let A be a bounded operator in K. Here, A is said to be *quotientable* with respect to K' if

$$AK' \subseteq K', \quad AK' \subseteq K''. \tag{5.22}$$

A is said to be *weakly quotientable* if the matrix elements $\langle \Psi_1, A\Psi_2 \rangle$, $\Psi_1, \Psi_2 \in K'$, depend only on equivalence classes of K'/K''. These definitions may be easily generalized to cover the case of unbounded operators. There is a unique operator $\hat{A}$ in K_{phys} associated with a quotientable operator A. If A is only weakly quotientable, the existence of $\hat{A}$ is guaranteed only in the case in which the space K'/K'' is complete.[24] In this case, $\hat{A}$ is constructed using the representation theorem for sesquilinear forms.[19] Let us come back to our concrete cases. It is evident that for a generic test function f

$$\phi(f)K_{z=0}' \not\subset K_{z=0}', \tag{5.23}$$

but it is not difficult to show that $\phi(f)$ is weakly quotientable when $f \in \mathscr{S}_0(\mathbf{R}^4)$ [the severe infrared singularities of the theory prevent the possibility to extend the quotiented field to functions belonging to $\mathscr{S}(\mathbf{R}^4)$]. The explicit expression of the quotiented field with respect to $K_{z=0}'$ is the following:

$$(\hat{\phi}(f)\hat{\Psi})^{(n)} = \frac{1}{2}\pi(n+1)^{1/2} \int [(1 - D)f(-k)]|_{C_+} \times \hat{\Psi}^{(n+1)}(k, k_1, \ldots, k_{n+1})\omega^{-3}\, d^3\mathbf{k} + (n)^{-1/2} \sum_{j=0}^{n} [(1 - D)f(k_j)]|_{C_+} \times \hat{\Psi}^{(n)}(k_1, \ldots, \not{k}_j, \ldots, k_n). \tag{5.24}$$

This expression gives a positive (noncovariant) quantization of the dipole field ($\Box^2\hat{\phi} = 0$) as an operator-valued distribution on $\mathscr{S}_0(\mathbf{R}^4)$, acting on a Hilbert space with positive metric. The fact that time translations are a broken symmetry now becomes more evident: Indeed, one may define a map γ_t in the polynomial algebra generated by the quotiented field $\hat{\phi}$:

$$\gamma_t(\hat{\phi}(f)) = \hat{\phi}(f_t), \tag{5.25}$$

with $f_t(x) = f(x_0 - t, \mathbf{x})$. It turns out that γ_t is no more a symmetry. The same holds for the Lorentz boosts.

From Eq. (5.24), one can easily obtain the quotient of the gauge invariant field $\Lambda = \Box\phi$. It is possible to find a nontrivial "vacuum sector" by applying polynomials of the quotiented gauge invariant field $\hat{\Lambda}$ to the vacuum vector (and completing with respect to $\langle\ ,\ \rangle$):

$$K_{\mathrm{vac},z=0} = \{ \overline{\mathscr{P}(\hat{\Lambda})\hat{\Psi}_0} \}. \tag{5.26}$$

This conclusion is in contrast with those of Refs. 7, 16, and 17. The explanation of this contrast is that while the vacuum expectation values of the polynomial algebra generated by Λ vanish, this is not the case for $\mathscr{P}(\hat{\Lambda})$ at the quotient and this because of the (5.23). It is worth mentioning that the map γ_t may be interpreted as time evolution in $K_{\mathrm{vac},z=0}$, and its representation is the usual one; for instance, if $\Psi \in K_{\mathrm{vac},z=0}^{(1)}$, one sees that the implementer of γ_t is given by

$$V(t)\Psi = \exp(ik_0 t)\Psi. \tag{5.27}$$

Therefore, starting from the local and covariant quantization of Sec. II, we have as a special case a positive quantization somewhat related to that exhibited in Ref. 4. The present derivation clarifies the general mechanism responsible for the peculiar features of their quantization; in particular, the time translations are implementable in the Krein space K, but not in K_{phys}. Here, we have another example (see also Ref. 14) supporting the advantages of the strategy of computing the Wightman functions (or equivalently solving the dynamics) in a local and covariant gauge, where a lot of symmetries are implementable and the theory has a linear structure. The physical interpretation of the model is then obtained simply by a linear subsidiary condition; it is at this stage that the physical structure, which is, in general, nonsymmetric, appears.

The physical space $K_{z=0,\mathrm{phys}}$ we have just constructed, may be regained easily using the canonical formalism introduced in the previous section. The Gupta–Bleuler condition now is written as follows:

$$a_2(\mathbf{k})|phys\rangle = 0. \tag{5.28}$$

It follows that $\hat{a}_2 = 0$, $\hat{a}_1 = a_1$. The quotiented field is given by

$$\begin{aligned}\hat{\phi}(t,\mathbf{x}) = (2\pi)^{-3/2} &\int \exp(i\omega t - i\mathbf{kx}) \\ &\times (1 - i\omega t)\hat{a}_1^\dagger(\mathbf{k})(2\omega^{3/2})^{-1} d^3\mathbf{k} \\ &+ (2\pi)^{-3/2} \int \exp(-i\omega t + i\mathbf{kx}) \\ &\times (1 + i\omega t)\hat{a}_1(\mathbf{k})(2\omega^{3/2})^{-1} d^3\mathbf{k}.\end{aligned} \tag{5.29}$$

The Hamiltonian is quotiented to zero. Again the time translations are not broken on the vacuum sector; their generator is the following:

$$H_v = \int \omega \hat{a}_1^\dagger(\mathbf{k})\hat{a}_1(\mathbf{k}) d^3\mathbf{k}. \tag{5.30}$$

On the other side, the space translations are implementable on the whole physical space and their generator is exactly the quotiented momentum:

$$\hat{P}^i = \int k^i \hat{a}_1^\dagger(\mathbf{k})\hat{a}_1(\mathbf{k}) d^3\mathbf{k}. \tag{5.31}$$

We note also that the equal time commutators involving quotiented fields which are not gauge invariant may depend explicitly on time.

It would now be interesting to know if there is the possibility of obtaining a positive quantization of the dipole field in which the time translations are an exact symmetry for the whole physical space and not only for the vacuum sector. This question has already been posed in literature by Narnhofer and Thirring.[4] The Krein space approach allows the possibility of giving an answer to this question. Indeed there are many other positive semidefinite subspaces of K and we may try to find some that are stable under time translations. Therefore, let us consider the following construction: Let $w = w(k)$ a complex-valued infinitely differentiable function such that

$$\mathrm{Re}\, w(k) = \mu > -1/2, \quad |\mathrm{Im}\, w(k)| < \mathrm{const}|k|. \tag{5.32}$$

The one-particle semidefinite subspace we are looking for is defined as the Krein completion $H_w^{(1)}$ of the dense set

$$\mathscr{G}_w^{(1)} = \{f \in \mathscr{S}_0(\mathbf{R}^4) : [(G - w(k))\tilde{f}(k)]|_{C_+} = 0\}, \tag{5.33}$$

where $G = k_1\partial/\partial k_1 + k_2\partial/\partial k_2 + k_3\partial/\partial k_3$. Again, H'_w is obtained by constructing the symmetric Fock space over $H_w^{(1)}$ and the physical space $H_{w,\mathrm{phys}}$ is given by H'_w/H''_w. In this case, we have

$$U(a)\mathscr{G}_w^{(1)} = \mathscr{G}_{w-i\mathbf{ka}}^{(1)}. \tag{5.34}$$

This implies that H'_w is not stable under space translations while it is stable under time translations, which, therefore, define an exact symmetry in $H_{w,\mathrm{phys}}$. As in precedence, we give the supplementary condition that characterizes the space $H'_{w=0}$:

$$\begin{aligned}&\phi^-(f)\Psi = 0, \quad \forall f \in \mathscr{S}_0(\mathbf{R}^4) \text{ such that} \\ &\qquad [(1 - \mathbf{D})\tilde{f}(-\mathbf{k})]|_{C_+} \\ &\qquad = -G[\tilde{f}(-k)|_{C_+}], \\ &\phi(v^-)\Psi = 0.\end{aligned} \tag{5.35}$$

Exactly as before the quotiented field may be constructed only for those test functions belonging to $\mathscr{S}_0(\mathbf{R}^4)$. We do not give here the complicated expression of the quotiented field but write its two-point function:

$$\begin{aligned}G(x-y) = W(x-y) + (32\pi^3)^{-1} &\sum_{i,j=1}^{3} x_i x_j \int k_i k_j \\ &\times \exp[ik(x-y)]|_{C_+} \omega^{-3} d^3\mathbf{k}.\end{aligned} \tag{5.36}$$

Thus we have obtained another (noncovariant) positive quantization of the dipole field for which the time translations are an exact symmetry of the physical space while the space translations are not. We remark that this quantization can never be obtained in a formal approach which exploits the usual creation and annihilation operators: Indeed, the supplementary condition (5.35) cannot be rewritten in terms of them.

Clearly the two quantizations that we have constructed must have the same physical meaning and indeed it is again possible to construct a "vacuum sector" in which the whole translation group is implementable and actually this vacuum sector is isomorphic to the previous one: This may be understood by looking at the Wightman functions of the gauge invariant quotiented fields that are the same in the two cases, as it may be directly verified using formulas (5.24) and (5.36).

VI. CONCLUDING REMARKS

We have come to the following conclusions: A local and covariant quantization of the dipole field model may only be obtained by making use of an indefinite metric space and it turns out that the most natural setting to discuss the model is the Krein space K, whose features have been described in Secs. II and III. Then, the thing to do is to look for a positive semidefinite subspace of K by means of constructing the physical space (and therefore the physical interpretation) of the model. In our case, we have seen that the infrared singularities of the Wightman functions forbid the possibility of constructing a Poincaré invariant physical space different from the vacuum vector. There is, however, the possibility to find subspaces of K that are not invariant under the Poincaré group and which originate physical spaces exhibiting its breaking (mechanism of confinement). In particular, we have constructed two explicit examples: In the first one, the time translations are broken while the space translations are an exact symmetry, and the contrary happens in the second one (actually other choices are possible but all exhibiting the breaking of the whole translation group). What is important is the fact that it is possible to construct a "vacuum sector" and this is the same in the two cases; therefore, the gauge

invariant content of the two positive quantizations that we have constructed is the same.

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On the asymptotics of finite energy solutions of the Yang–Mills–Higgs equations

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Using *a priori* estimates by Taubes [A. Jaffe and C. H. Taubes, *Vortices and Monopoles* (Birkhauser, Boston, 1980)] on the rate of decay of finite energy solutions of the Yang–Mills–Higgs equations, the limits of the solution fields are proven to exist at infinity. As expected, the limit of the gauge field is a pure Yang–Mills field on the reduction bundle over S^2 defined by the limit of the Higgs field.

I. INTRODUCTION

We give a detailed proof of a fact conjectured by physicists a long time ago.[1]

Consider any finite energy solution (A,Φ) of the Yang–Mills–Higgs equations on $\mathbb{R}^3$:

$$d_A{}^*F_A = [d_A\Phi,\Phi],$$

$$d_A{}^*d_A\Phi = (\lambda/2)(|\Phi|^2 - 1)\Phi.$$

Then A becomes a pure U(1)–Yang–Mills connection on the "sphere at infinity." For a physicist this means that at large atomic scales all that is left from a non-Abelian t'Hooft–Polyakov monopole is an Abelian Dirac monopole. This was one of the main reasons for introducing the theory, after all. For a survey see Taubes.[2]

Now it is well known that the holonomy of a Yang–Mills field on the sphere is either $\mathbb{R}$ or U(1), see Atiyah and Bott[3] and Friedrich and Habermann.[4] Starting with a compact gauge group immediately excludes $\mathbb{R}$. On the other hand, a connection always reduces to its holonomy bundle. The conjecture then is that any finite energy monopole becomes a pure Yang–Mills field at infinity. [In the case we study here, $G = \mathrm{SU}(2), H = U(1)$. The above complication is not apparent since we prove directly that the limit is a U(1)–Yang–Mills field.]

Of course, the first thing one has to make sense of is what exactly is meant by "sphere at infinity." Since $\mathbb{R}^3\setminus\{0\}$ is $S^2\times(0,\infty)$ only topologically but not metrically, some care has to be taken. In fact, we have found this point to be a major step in the proof.

The idea is that the sphere at infinity should be interpreted as a family of configurations on the fixed unit sphere S^2 in $\mathbb{R}^3$ with its standard Riemannian metric. This family is parametrized by r, the distance from the origin in $\mathbb{R}^3$. The limits at infinity are nothing but the limits of the family as the parameter tends to infinity. This does not influence the calculations for the Higgs field at all, since we deal with limits of functions. It does, however, clarify the form part of the configuration, where the Riemannian structure comes to the fore.

Morally speaking if $d_A\Phi$ decays to zero the first of the equations above should give the Yang–Mills equation:

$$d_A{}^*F_A = 0.$$

It is this observation one has to make sense of. For this, we have found that the Sobolev spaces of fields over S^2 are the appropriate setting: although one starts with solutions, therefore smooth objects, some differentiability is lost by passing to the limit. Such a limit can be realized only in a Sobolev space.

Having realized these two points, the rest of the proof relies on Taubes' estimates in Taubes[5] and Jaffe and Taubes,[6] Uhlenbeck's weak compactness theorem,[7] and a formula by Taubes as it appears here. The rest consists of analytic pleasantries.

Finally, viewing the problem as the behavior of solutions to a system of partial differential equations, with the finite energy condition replacing boundary values, we see that monopoles behave quite differently than harmonic functions for example, see Anderson and Schoen.[8] However, for the Bogomol'nyi case (the minima of the $\lambda = 0$ case) with hyperbolic metric the conjecture is no longer true, see Braam and Austin.[9]

After quickly going over the basic definitions of the theory in Sec. II, we prove the existence of limits for the Higgs part of finite energy configurations in Sec. III. In the same section we also describe the symmetry breaking in terms of reductions of bundles, a more or less standard procedure. Section IV first states Taubes' estimates for finite energy solutions for the SU(2) case. These are used to prove the existence of limits for the gauge part of a solution. Using the same estimates, it is easy to see that the limit connection reduces to the subbundle defined by the Higgs part of the solution. Section IV shows why this limit connection is coclosed, i.e., a U(1)–Yang–Mills field on S^2. Here, we have to use a formula by Taubes. We explain how to derive the formula in the Appendix.

Apart from Sec. III, we concentrate on the case with gauge group SU(2). As it will become clear, the same results would hold for any gauge group G and any small group H if we knew that the estimates of Theorem 4.1 were true in this generality. For the case when H is an Abelian subgroup of G one recovers most of the estimates, see Taubes,[10] using more or less the same techniques as in Jaffe and Taubes.[6] However, further analysis needs to be carried out when H is not Abelian.

II. THE YANG–MILLS–HIGGS EQUATIONS

The mathematical setting for the Yang–Mills–Higgs theory is provided by connections A on a principle G bundle

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P over $\mathbb{R}^3$ and a sections Φ of an associated bundle $P\times_G L$. Here, L is a finite dimensional, inner product space on which G, a compact Lie group, acts orthogonally. The group of gauge transformations acts on pairs (A,Φ) by

$$(g,(A,\Phi))\to(gAg^{-1}+g\,dg^{-1},g\cdot\Phi).$$

The Lagrangian of the theory is to be viewed as a gauge invariant functional on such pairs (A,Φ) given by

$$\mathrm{YMH}(A,\Phi)=\int_{\mathbb{R}^3}\left\{\frac{1}{2}|F_A|^2+\frac{1}{2}|d_A\Phi|^2+V(\Phi)\right\}d^3x.$$

Here, F_A is the curvature of A, $d_A\,\Phi$ is the covariant derivative, and V a Higgs potential satisfying the following properties: (a) It is smooth, non-negative, and G-invariant function defined on the representation space L. (b) It gives symmetry breaking, that is, it achieves the minimum value zero on a single nontrivial orbit, the vacuum. For future use, let H denote the (uniquely determined up to conjugation) isotropy group of this orbit. (Other conditions usually imposed on V, such as renormalizability conditions, are of no relevance here.)

The configurations (A,Φ) are usually taken to be in the corresponding $L^2{}_{1,\mathrm{loc}}$ section spaces. This, and the definition of the action forces the gauge transformations to be in $L^2{}_{2,\mathrm{loc}}(\mathbb{R}^3,G)$. However, it is a theorem of Taubes[6] that such a solution (A,Φ) of the corresponding Euler–Lagrange equations

$$d_A{}^*F_A=-\sum_i\langle t(\xi_i)\cdot\Phi,d_A\Phi\rangle\xi_i, \qquad \text{(YMH1)}$$

$$d_A{}^*d_A\Phi=\frac{\partial V}{\partial\Phi} \qquad \text{(YMH2)}$$

is always gauge equivalent to a smooth pair if its energy $\mathrm{YMH}(A,\Phi)$ is finite. Hence, whenever interested in finite energy solutions only, we shall always start with smooth (A,Φ).

The case that is mostly studied is for $G=\mathrm{SU}(2)$, acting on its Lie algebra via the adjoint representation. For Higgs potential one then takes $V(\Phi)=\lambda/2(|\Phi|^2-1)^2$, the vacuum orbit then being the unit sphere in the Lie algebra and $H=\mathrm{U}(1)$. The equations can then be written exactly as in the Introduction.

III. FINITE ENERGY CONFIGURATIONS: THE GENERAL CASE

We present here some preliminary results concerning the asymptotics of finite energy fields. In particular, we are not assuming that the fields solve any equations. We are assuming the structure group G to be any compact Lie group, the small group H to be any subgroup of G and V to be any symmetry breaking Higgs potential. It turns out that much more can be said about the Higgs field Φ than the gauge potential A. In the next chapter, where we specialize to solutions for $G=\mathrm{SU}(2)$ and $H=\mathrm{U}(1)$, we can deal with the asymptotics of A using known estimates for F_A.

By configuration we mean a pair (A,Φ) with both members of the pair in the corresponding $L^2{}_{1,\mathrm{loc}}$ spaces and such that the energy is finite. We use spherical coordinates (r,θ,φ) with $0\leqslant r$, $0\leqslant\theta\leqslant\pi$, $0\leqslant\varphi\leqslant2\pi$ on $\mathbb{R}^3$ so that the volume element on $\mathbb{R}^3$ is $r^2\sin\theta\,dr\,d\theta\,d\varphi$ and the metric is $ds^2=dr^2+r^2\,d\theta^2+r^2\sin\theta\,d\varphi^2$. An orthonormal basis for the cotangent space at a point is then given by

$$\{dr,r\,d\theta,r\sin\theta\,d\varphi\}.$$

We write $d\Omega$ for the volume element of the unit sphere, $d\Omega=\sin\theta\,d\theta\,d\varphi$.

Lemma 3.1: If Φ is in $L^2{}_{1,\mathrm{loc}}$ then Φ is continuous in almost any radial direction.[11]

Proof: Since Φ is in $L^2{}_{1,\mathrm{loc}}$, Φ is in $L^2{}_1$ on the annulus $\{x:1\leqslant|x|\leqslant R_n\}$ for $R_n>1$. Therefore, in spherical coordinates we have that

$$\int_{S^2}\int_1^{R_n}r^2(|\Phi|^2+|d\Phi|^2)dr\,d\Omega$$

is finite. This means that in almost any radial direction the integral

$$\int_1^{R_n}r^2(|\Phi|^2+|d\Phi|^2)dr$$

and since $r\geqslant1$ the integral

$$\int_1^{R_n}(|\Phi|^2+|d\Phi|^2)dr,$$

is finite, too. Hence, Φ is in $L^2{}_1$ in almost any radial direction within the annulus. By Sobolev's embedding theorem for dimension 1, Φ is continuous in each such direction. Taking an increasing sequence of R_n's so as to cover the whole of $\mathbb{R}^3$ and forgetting each time a set of measure zero, we end up with almost all radial directions on each of which Φ is continuous.

One of the major technical problems when dealing with the coupling term $d_A\Phi$ of the Lagrangian is that it involves both the Φ and the A field and therefore, in general, gives information for none of them unless something is known about one of them. This difficulty can be avoided for the radial components when working in the radial gauge, which is characterized by the condition $\Sigma x_iA_i=0$ or, in terms of the spherical coordinates of the connection form, $A_r=0$. For the existence of such gauges see the next section. We use such a gauge in the following proposition.

Proposition 3.2: Let (A,Φ) be a finite energy configuration (not necessarily a solution). Then in a radial gauge Φ achieves a limit in almost any radial direction.

Proof: The finite energy condition means that $\|d_A\Phi\|_2$ is finite. Written out in a radial gauge this gives

$$\int_{S_2}\int_0^\infty\{r^2|\partial_r\Phi|^2+|\partial_\theta\Phi+[A_\theta,\Phi]|^2+\sin\theta^{-2}|\partial_\varphi\Phi+[A_\varphi,\Phi]|^2\}dr\,d\Omega<\infty.$$

Then for almost any radial direction

$$\int_0^\infty r^2|\partial_r\Phi|^2\,dr$$

is finite.

Pick a generic radial direction $(\cdot,\omega_0)$ in $\mathbb{R}^3$ for which this integral is finite and the previous lemma is true and two points (R_1,ω_0) and (R_2,ω_0) with $R_1<R_2$. On such a direction, using Holder's inequality and the continuity of Φ, we have

$$
\begin{aligned}
&|\Phi(R_1,\omega_0)-\Phi(R_2,\omega_0)| \\
&\quad\leqslant\int_{R_1}^{R_2}|\partial_r\Phi(r,\omega_0)|\,dr \\
&\quad\leqslant\left(\int_{R_1}^{R_2}\frac{1}{r^2}\,dr\right)^{1/2}\left(\int_{R_1}^{R_2}r^2|\partial_r\Phi(r,\omega_0)|^2\,dr\right)^{1/2} \\
&\quad\leqslant M\left(\frac{1}{R_1}-\frac{1}{R_2}\right)^{1/2}.
\end{aligned}
$$

Therefore, for each such radial direction the Higgs field has a limit as the distance from the origin tends to infinity.

Notice that the constant M in the proof of the proposition depends on the direction and hence the estimate is not uniform.

Let $\Phi_\infty(\omega)$ denote the limit on the radial direction (r,ω) of the Higgs field Φ as r tends to infinity whenever this limit exists. Exploiting the finite energy condition through the third term in the Lagrangian gives that

$$
\int_{S_2}\int_0^\infty r^2\sin\theta V(\Phi(r,\omega))dr\,d\omega<\infty.
$$

Therefore,

$$
\int_0^\infty r^2V(\Phi(r,\omega))dr
$$

is finite for almost any radial direction ω.

Since $\Phi(r,\omega)$ has a limit as r tends to infinity and V is at least continuous, $V(\Phi(r,\omega))$ must go to zero as r tends to infinity, for the last integral to be finite. But V achieves the value 0 only on the vacuum orbit, therefore Φ_∞ defines a map

$$
\Phi_\infty: S^2\to G/H.
$$

Such a map defines a reduction of any trivial G bundle over S^2 to an H subbundle in the following way: It is well known that reductions of a G bundle P to H subbundles are in one to one correspondence with sections of the associated bundle

$$
Q=P\times_G G/H\approx P/H.
$$

Here, G acts on the quotient space by left multiplication, see Kobayashi and Nomizu.[12] In our case P is trivial and hence isomorphic to $S^2\times G$. Using this identification, the bundle Q is isomorphic to $S^2\times G/H$ via the following isomorphism:

$$
[(\omega,g),g'H]\mapsto(\omega,gg'H).
$$

It is then clear that a map like Φ_∞ defines a section of $S^2\times G/H$, hence a section of Q and therefore a reduction of P to an H bundle.

We have deliberately avoided any adjectives like smooth, continuous, and the similar. As we are going to prove in the next section, Φ_∞ is continuous when dealing with solutions and therefore the reduction will be within the known framework. We just mention here that measurable reductions of bundles have been studied, see Zimmer.[13] This kind of analysis together with the methods of Uhlenbeck[14] for Sobolev connections should give a way of defining a magnetic charge in the general setting as a generalized characteristic class of some measurable reduction.

IV. G=SU(2), ADJOINT REPRESENTATION: THE ASYMPTOTICS OF A FINITE ENERGY SOLUTION

Taubes[5,6] proves the following for the adjoint SU(2) case.

Theorem 4.1: Let (A,Φ) be a smooth finite energy solution of the Yang–Mills–Higgs equations. Then we have the following *a priori* estimates.

Coupling term estimate: there exists a positive constant m and for any positive ϵ there exists a positive real number $M(\epsilon)$ such that

$$
|d_A\Phi|(x)\leqslant M(\epsilon)e^{-(1-\epsilon)m|x|}.
$$

Higgs field estimate:

$$
0\leqslant 1-|\Phi|\leqslant M(\epsilon)e^{-(1-\epsilon)m|x|}.
$$

Curvature estimate: there exists a constant M such that for x with $|x|$ sufficiently large

$$
|F_A|(x)\leqslant M(1+|x|^2)^{-1}.
$$

In particular, we have for the transverse to Φ components:

$$
|[F_A,\Phi]|\leqslant M(\epsilon)e^{-(1-\epsilon)|x|}.
$$

Equipped with these estimates, start in a gauge where the solution configuration (A,Φ) is smooth on $\mathbb{R}^3$. Gauge transform to a radial gauge using a smooth gauge transformation, which we can obtain by solving the following ordinary differential equation for $g(\cdot,\varphi,\theta)$:

$$
\begin{aligned}
&g^{-1}(r,\varphi,\theta)A_r(r,\varphi,\theta)g(r,\varphi,\theta) \\
&\quad+g^{-1}(r,\varphi,\theta)\partial_r g(r,\varphi,\theta)=0,
\end{aligned}
$$

with some initial conditions. We are then in a gauge where A and Φ are smooth and

$$
A_r=\sum x_iA_i=0.
$$

We shall now see how the connection part of the configuration behaves in this gauge. Let

$$
i_R: S^2\to\mathbb{R}^3
$$

be the family of embeddings that send the point (φ,θ) of the sphere to (r,φ,θ) in $\mathbb{R}^3$. Using them to pull back the bundle P and the connection A we have the one parameter family $i_R{}^*(P)$ of bundles over S^2, all equivalent to the trivial one, each supplied with the connection $i_R{}^*(A)$. Since we are in a radial gauge and we can write A over $\mathbb{R}^3$ as

$$
A(r,\varphi,\theta)=A_\varphi(r,\varphi,\theta)d\varphi+A_\theta(r,\varphi,\theta)d\theta,
$$

on the sphere we have that

$$
i_R{}^*(A)(\varphi,\theta)=A_\varphi(R,\varphi,\theta)d\varphi+A_\theta(R,\varphi,\theta)d\theta.
$$

From now on we write A_R for $i_R{}^*(A)$ when there is no confusion and

$$
A_R=(A_R)_\varphi(\varphi,\theta)d\varphi+(A_R)_\theta(\varphi,\theta)d\theta.
$$

That is, we want to view the r variable in $\mathbb{R}^3$ as a parameter for S^2. The respective curvatures F_{A_R} on S^2 are

$$
F_{A_R}(\varphi,\theta)=F_{\varphi\theta}(R,\varphi,\theta)d\varphi\wedge d\theta,
$$

where

$$
\begin{aligned}
F_A(r,\varphi,\theta)=&F_{\varphi\theta}(r,\varphi,\theta)d\varphi\wedge d\theta+F_{r\theta}(r,\varphi,\theta)dr\wedge d\theta \\
&+F_{r\varphi}(r,\varphi,\theta)dr\wedge d\varphi
\end{aligned}
$$

on $\mathbb{R}^3$.

The curvature estimate of Theorem 4.1 then gives that

$$|F_{\varphi\theta}(r,\varphi,\theta)d\varphi\wedge d\theta|\leqslant M(1+r^2)^{-1}.$$

An orthonormal basis for the cotangent space of $\mathbb{R}^3$ at the point (r,φ,θ) is given by

$$\{dr, r\sin\theta\, d\varphi, r\, d\theta\}.$$

Therefore,

$$\begin{aligned}|r^{-2}\sin\theta^{-1}F_{\varphi\theta}(r,\varphi,\theta)| &= |r^{-2}\sin\theta^{-1}F_{\varphi\theta}(r,\varphi,\theta)(r\sin\theta)d\varphi\wedge r\,d\theta| \\ &\leqslant M(1+r^2)^{-1},\end{aligned}$$

which gives that

$$|\sin\theta^{-1}F_{\varphi\theta}(r,\varphi,\theta)|\leqslant M$$

or

$$|F_{A_R}(\varphi,\theta)|\leqslant M,$$

for all R.

That is, the A_R's are connections with uniform bounds on the curvature in the sense of Uhlenbeck.[7] This provides us with an elegant, if somewhat sophisticated, way of finding the limit of $\{A_R\}$. We know of no other way.

The main result in Uhlenbeck[7] is the following theorem.

Theorem 4.2: Let M be a compact manifold of dimension M and $\{A_n\}$ a sequence of connections on a bundle P over M, in $L^p{}_1(M)$ with $2p>n$. If there exists a constant B such that

$$\|F_{A_n}\|_{L^p}\leqslant B$$

then there exists a subsequence $\{A_{n_i}\}$ of $\{A_n\}$ and a sequence $\{g_{n_i}\}$ of gauge transformations in $L^p{}_2(M)$ with the property: $g_{n_i}\cdot A_{n_i}$ converges weakly to a connection A in $L^p{}_1(M)$.

It is part of the proof of the theorem that A defines a connection on a bundle isomorphic to the original P. For $p=2n$ this is no longer the case, see Sedlacheck.[15] In our case, we have that $M=S^2$ and then $n=2$. The family of connections is smooth and therefore each of them is in the $L^p{}_1(S^2)$ Sobolev space required by the theorem, for any p. To avoid any ambiguity concerning the limit connection we take the sequence on which to apply the theorem to be $\{A_R\}$ for all positive integers R. Then the A_R's live on bundles that are equivalent to the trivial one and the theorem applies with $B=M$. We call the weak limit connection A_∞. It lives on the trivial bundle over S^2 and is in $L^p{}_1(S^2)$, for $p>1$. Of course, we rename the subsequences to $\{A_R\}$ and $\{g_R\}$.

To make sure that we are still within the configuration space we have chosen, we want to realize the corresponding gauge in $\mathbb{R}^3$. Define $g:\mathbb{R}^3\to G$ by

$$g(r,\varphi,\theta)=g_R(\varphi,\theta)$$

when r is in the strip

$$[(R-1)+R]/2<r<[(R+1)+R]/2.$$

If we take $p=2$, each g_R is $L^2{}_2$ on the sphere and g is $L^2{}_2$ on the strips. Using a bump function identically 1 on the narrower strips

$$(4R-1)/4<r<(4R+1)/4,$$

it is clear that we can join things together so that g is $L^2{}_{2,\mathrm{loc}}$. The resulting configuration then on $\mathbb{R}^3$ is gauge equivalent to the original one via one of the gauge transformations of the theory. This is the gauge we wish to work in.

We now want to prove that the limit of the Higgs field in this gauge is continuous and therefore defines a reduction to a U(1) subbundle as explained in Sec. III. We shall also prove that the limit connection reduces to this subbundle, or, to use a piece of terminology from Physics, the finite energy condition is satisfied. (It is well known that in a radial gauge Φ has a continuous limit at infinity, see Jaffe and Taubes,[6] p. 38. The problem here is that since the gauge transformations g_R in $L^p{}_2$ do not necessarily have a limit we cannot conclude immediately that the limit of Φ in the final gauge exists.)

We claim that Φ_R has a pointwise limit Φ_∞ in the gauge where A_∞ exists. For this, first notice that since $|\Phi|\leqslant 1$, $\{\Phi_R\}$ is bounded in any $L^p(S^2)$, for any p:

$$\|\Phi_R\|_p\leqslant(\mathrm{vol}(S^2))^{1/p}.$$

This is true for any gauge, since $|\Phi|$ is a gauge invariant quantity. Now it is a standard fact that in a reflexive space bounded sets are weakly compact. Therefore, in any gauge Φ_R has a subsequence that converges weakly in L^p, for any $p\geqslant 2$.

We also have that A_R converge weakly to A_∞ in $L^p{}_1$ for all p. By the Rellich–Kondrachov theorem, they converge strongly in L^q for $q\geqslant 1$, and therefore (up to subsequences) pointwise. In particular, A_R is bounded in L^q, $q\geqslant 1$.

Then $[A_R,\Phi_R]$ is bounded in L^q, too: using the elementary inequality

$$|[A_R,\Phi_R]|^2+|\langle A_R,\Phi_R\rangle|^2=|A|^2|\Phi_R|^2,$$

we see that

$$|[A_R,\Phi_R]|\leqslant|A_R||\Phi_R|\leqslant|A_R|.$$

Applying this for $p=2$ we have that $[A_R,\Phi_R]$ converges weakly to a limit B_∞ in L^p. (We shall prove in a while that this limit is independent of p.)

Now use the coupling term estimate of Theorem 1: The exponential decay of $|d_A\Phi|$ on $\mathbb{R}^3$ means that $|d_{A_R}\Phi_R|\to 0$ on S^2, much faster than R^{-1}. Hence, $d_{A_R}\Phi_R\to 0$ in any L^p strongly.

Then

$$d(\Phi_R)+[A_R,\Phi_R]\to 0$$

and

$$[A_R,\Phi_R]\to B_\infty \text{ weakly}$$

give that

$$\partial_{\varphi,\theta}\Phi_r\to -(B_\infty)_{\varphi,\theta} \tag{4.1}$$

in L^p, weakly. Notice that Φ_R are differentiable since we started from a smooth gauge and transformed by $L^p{}_2$, that is C^1 if $p>2$, transformations. This means that Φ_R has a weak limit in $L^p{}_1(S^2)$. Let Φ_∞ denote this limit. [Naive proof: For a smooth function f on the sphere we have that

$$\begin{aligned}\int\langle\partial_{\varphi,\theta}\Phi_R, f\rangle &= -\int\langle\Phi_R,\partial_{\varphi,\theta}f\rangle\to -\int\langle\Phi_\infty,\partial_{\varphi,\theta}f\rangle,\end{aligned}$$

while

$$\int \langle \partial_{\varphi,\theta} \Phi_R f\rangle \to \int \langle (B_\infty)_{\varphi,\theta} f\rangle,$$

which gives that

$$\int \langle \Phi_\infty, \partial_{\varphi,\theta} f\rangle = -\int \langle (B_\infty)_{\varphi,\theta} f\rangle.\Big]$$

Since Φ_R converges weakly in $L^p{}_1$ for $p\geqslant 2$, it converges strongly in L^q for $q\geqslant 1$. In particular, its weak limits in L^p for $p\geqslant 2$ are its pointwise limit and the weak limit B_∞ of $[A_R,\Phi_R]$ is nothing but the pointwise limit $[A_\infty,\Phi_\infty]$.

This has the following two consequences: First, the limit of the Higgs field in the final gauge is continuous: Taking $p=3$ in Eq. (4.1), for example, we have that Φ_∞ lies in $L^3{}_1$ and hence is continuous. Second, Eq. (4.1) shows that $d\Phi_\infty$ is $-[A_\infty,\Phi_\infty]$. That is, we have the reduction (finite energy) condition:

$$d_{A_\infty}\Phi_\infty = 0.$$

As an elementary instance of bootstrapping, notice that by embedding theorems again A_∞ is continuous and since we just proved that Φ_∞ is continuous we have that the derivatives of Φ_∞ are continuous, therefore Φ_∞ is C^1. Therefore, the finite energy condition holds in a strong sense. Summarizing, we have the following for the SU(2)-adjoint case.

Theorem 4.3: Every finite energy solution is gauge equivalent to a smooth solution (A,Φ) with the following properties. (a) The connections A_R on the trivial bundle over S^2 converge to a connection A_∞ on the same bundle. The convergence is strong in $L^p(S^2)$ and weak in $L^p{}_1(S^2)$. In any case A_∞ is continuous. (b) The Higgs fields converge pointwise to Φ_∞ and weakly in $L^p{}_1(S^2)$ and Φ_∞ is at least C^1. (c) A_∞ and Φ_∞ satisfy the finite energy condition $d_{A_\infty}\Phi_\infty = 0$.

Recall now the discussion on the reduction of the previous section. Since in the case we are studying the Higgs potential is given by $V(\Phi) = (|\Phi|^2 - 1)^2$, the small group of the theory is U(1). Therefore, Φ_∞ defines a reduction of the trivial bundle over S^2 on which A_∞ is defined, to a U(1) subbundle. The meaning of the finite energy condition is that A_∞ reduces on this subbundle. That is, its restriction on the subbundle is a U(1) connection. (Recall[12] that, given a section s of the associated bundle $P\times_G G/H$ defining a reduction of the G bundle P to an H bundle S, a given connection A on P reduces to S if and only if s is parallel with respect to A.)

We would like to remark here that the finite energy condition is a geometrical way of proving something that ought to be provable using analysis: Since A_∞ reduces to a U(1) connection only the corresponding U(1) components of A on $\mathbb{R}^3$ survive and the rest fade away. In terms of massive and massless components, one should be able to form appropriate equations that would give exponential decay to all the components but the ones corresponding to the U(1) subgroup. The major technical problem is that we do not know of any global gauge on $\mathbb{R}^3$ in which the Yang–Mills–Higgs equations are elliptic for A. Only local gauges are known to exist in which the extra condition d^*A is satisfied. In fact, these are the gauges used by Uhlenbeck in her weak compactness theorem.

V. A_∞ IS YANG–MILLS

We shall now show that the reduced connection is Yang–Mills.

First recall that the curvature form for the connection induced by A_∞ on the subbundle defined by the Φ_∞ section is given [up to a multiple of $\sqrt{(-1)}$] by

$$\langle F_{A_\infty},\Phi_\infty\rangle + \langle [d_{A_\infty}\Phi_\infty, d_{A_\infty}\Phi_\infty],\Phi_\infty\rangle,$$

see for example Madore.[17] The same formula appears also in Schwarz.[18] By the finite energy condition we are left with

$$\langle F_{A_\infty},\Phi_\infty\rangle.$$

This is the curvature of the reduced connection since by definition a connection that reduces equals its induced connection. It is here that we need Taubes' formula.

Proposition 5.1: On $\mathbb{R}^3$,

$$\langle F_A,\Phi\rangle = C\,dS^2 + \omega,$$

where dS^2 is the area element of the unit sphere in $\mathbb{R}^3$ and ω is a real valued two-form on $\mathbb{R}^3$ with $|(\partial_r)^k\omega| \leqslant r^{-3-k}$.

We give a proof of this in the Appendix. Now every constant multiple of dS^2 is a Yang–Mills curvature. Since ω decays to zero, the formula shows that at large distances we are left only with a Yang–Mills field. However, it does not explain why only the $\langle F_A,\Phi\rangle$ part is relevant, or why this limit is actually realized on a bundle "at infinity." Using it, we finally prove the following theorem.

Theorem 5.2: $\langle F_{A_\infty},\Phi_\infty\rangle$ is a pure Yang–Mills solution on the sphere.

Proof: From Taubes' formula we see that $\langle F_{A_R},\Phi_R\rangle$ converges to $C\,dS^2$ strongly in any $L^p(S^2)$

$$\langle F_A,\Phi\rangle = C\,dS^2 + \omega$$

on $\mathbb{R}^3$, gives that

$$\langle F_{A_R},\Phi_R\rangle = C\,dS^2 + \omega_{\varphi\theta}(R,\cdot)\,d\varphi\wedge d\theta.$$

Since $|\omega| \leqslant |x|^{-3}$ on $\mathbb{R}^3$, $|\omega_{\varphi\theta}(R,\cdot)| \leqslant R^{-1}$ on S^2. Hence, $\langle F_{A_R},\Phi_R\rangle - C\,dS^2$ tends to zero in any L^p norm. Notice that this is a gauge invariant statement.

We want to argue that in our gauge the limit of $\langle F_{A_R},\Phi_R\rangle$ is actually $\langle F_{A_\infty},\Phi_\infty\rangle$. Since A_R converges weakly to A_∞ in $L^p{}_1$ it follows that F_{A_R} converges weakly to F_{A_∞} in L^p, but this does not seem to be enough to prove that $\langle F_{A_R},\Phi_R\rangle$ converges in any sense to $\langle F_{A_\infty},\Phi_\infty\rangle$. We present here a somewhat indirect argument: As argued above, $\langle F_{A_R},\Phi_R\rangle$ has a pointwise limit and, in the gauge we are working in, so does Φ_R, see above. Therefore, $|\Phi_R|^{-2}\langle F_{A_R},\Phi_R\rangle\Phi_R$ has a pointwise limit. (We also use the fact that $|\Phi_R|$ tends to 1, another gauge invariant argument.)

Similarly, from the estimate on the transverse components of Theorem 4.1,

$$|\Phi_R|^{-2}[\Phi_R,[\Phi_R,F_{A_R}]]$$

has a pointwise limit zero. Since this accounts for the whole of the curvature, F_{A_R} has a pointwise limit which of course has to be equal to its weak L^p limit, F_{A_∞}, by the uniqueness of a weak limit. Here, we use the standard fact that a bounded sequence in L^p with pointwise limit converges weakly to this

limit for $p \geqslant 2$, see Aubin.[19] Then $\langle F_{A_R}, \Phi_R \rangle$ converges pointwise to $\langle F_{A_\infty}, \Phi_\infty \rangle$ (therefore, also weakly and strongly) and hence $\langle F_{A_\infty}, \Phi_\infty \rangle = C\, dS^2$.

Remark: Had we chosen some other sequence of A_R's they would still have the same curvature on the reduced bundle, as the theorem shows. Then their limits on the reduced bundle would be gauge equivalent: for any two connections A_1 and A_2 on the sphere with $dA_1 = dA_2$ we have $A_1 = A_2 + g\, dg^{-1}$, $g = \exp f$ with $df = A_1 - A_2$.

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APPENDIX: THE ASYMPTOTIC FORMULA

We describe how one proves the formula as we learned it from Taubes.[20] Basic ideas of the estimates for a slightly more complicated situation in the Prasad–Sommerfield limit can be found also in Taubes.[21]

One starts with the real valued one-form $\alpha = \langle \Phi, *_E F_A \rangle$ on $\mathbb{R}^3$. The Bianchi identity and the first Yang–Mills–Higgs equation give

$$\begin{aligned} d *_E \alpha &= d *_E \langle \Phi, *_E F_A \rangle \\ &= d \langle \Phi, F_A \rangle = \langle d_A \Phi \wedge F_A \rangle + \langle \Phi, d_A F_A \rangle \\ &= \langle d_A\, \Phi \wedge F_A \rangle = :p \end{aligned}$$

and

$$\begin{aligned} *_E d\alpha &= *_E d \langle \Phi, *_E F_A \rangle \\ &= *_E \langle d_A \Phi \wedge *_E F_A \rangle + *_E \langle \Phi, d_A *_E F_A \rangle \\ &= *_E \langle d_A \Phi \wedge *_E F_A \rangle + \langle \Phi, *_E d_A *_E F_A \rangle \\ &= *_E \langle d_A \Phi \wedge *_E F_A \rangle = :q, \end{aligned}$$

respectively. Note that once again the coupling term estimate and the curvature estimate give that both p and q have exponentially decaying lengths.

We now define the operator

$$L: \Omega^0(\mathbb{R}^3) \oplus \Omega^1(\mathbb{R}^3) \to \Omega^0(\mathbb{R}^3) \oplus \Omega^1(\mathbb{R}^3),$$

by

$$L(f,\beta) = (d *\beta, df + *_E d\beta).$$

In Taubes' quaternionic notation, if

$$\Psi = (f,\beta) = \Psi_0 + \Sigma \Psi_i \tau_i$$

with $\Psi_0 = f$ and $\Psi_i = \beta_i$, the formula for L becomes

$$L(\Psi) = \sum (\partial_i \Psi) \tau_i,$$

where quaternionic multiplication is meant.

We can then write the equations above in a compact form as

$$L(0,\alpha) = (*_E p, q).$$

The main point now is that L is in a sense the square root of the Laplacian on $\Omega^0(\mathbb{R}^3) \oplus \Omega^1(\mathbb{R}^3)$:

$$\begin{aligned} L^2(f,\beta) &= L(d *\beta, df + *_E d\beta) \\ &= (d * df, dd *\beta + *_E d *_E d\beta) \\ &= (d * df, dd *\beta + d * d\beta) \\ &= (-\Delta f, -\Delta \beta). \end{aligned}$$

Here, we have used that on two-forms over $\mathbb{R}^3$

$$*_E d *_E = d *$$

and Δ denotes the Laplacian both on functions and forms.

One uses this observation to write a Green's function for L and therefore a formula for α. Following the quaternionic notation, since $L(0,\alpha) = (*p, q)$ and since Green's function for the Laplacian on $\mathbb{R}^3$ is $|x-y|^{-1}$,

$$\begin{aligned} (0,\alpha)(x) &= \sum_i a_i(x) \tau_i \\ &= -\int_{\mathbb{R}^3} L(|x-y|^{-1}, 0) \left(*p + \sum_i q_i \tau_i \right) \\ &= -\int_{\mathbb{R}^3} \left(0, \sum_i \frac{x_i - y_i}{|x-y|^3} \tau_i \right) \left(*p + \sum_i q_i \tau_i \right) \\ &= \int_{\mathbb{R}^3} \left(\sum_i \frac{x_i - y_i}{|x-y|^3} q_i, -\sum_i \frac{x_i - y_i}{|x-y|^3} \right) \\ &\quad \times *p \tau_i - \sum_{ij} \frac{x_i - y_i}{|x-y|^3} \tau_i q_j \tau_j, \end{aligned} \tag{A1}$$

where quaternionic multiplication is implied.

The way to prove this is similar to the way one proves that the unique solution that vanishes at infinity for the equation

$$\Delta u = \nabla f$$

is given by the formula:

$$u(x) = \int_{\mathbb{R}^3} d\, |x-y|^{-1} f(y) dy,$$

see the last chapter of Jaffe and Taubes.[6] The decay of the fields guaranties that the integrals are finite.

The first thing that Eq. (A1) implies is that

$$\int_{\mathbb{R}^3} \sum_i \frac{x_i - y_i}{|x-y|^3} q_i(y) dy = 0.$$

Now use the multipole expansion

$$\frac{x_i - y_i}{|x-y|^3} = \frac{x_i}{|x|^3} - \frac{y_i}{|x|^3} + \cdots = \frac{x_i}{|x|^3} + (|x|^{-3}).$$

We then have that for all x in $\mathbb{R}^3$

$$\sum_i \int_{\mathbb{R}^3} \frac{x_i}{|x|^3} q_i(y) dy - O(|x|^{-3}) \sum_i \int_{\mathbb{R}^3} F(y) q_i(y) dy = 0. \tag{A2}$$

Notice that we have enough decay on q so that the last integral is finite no matter what power of y appears in the integrand. Now choose $x = (t,0,0)$, $t > 0$. Then (A2) becomes

$$\int_{\mathbb{R}^3} |t|^{-2} q_1(y) dy + O(|t|^{-3}) \sum_i \int_{\mathbb{R}^3} F(y) q_i(y) dy = 0.$$

Multiplying by $|t|^2$ and letting t tend to infinity we have

$$\mathbb{R}^3 q_1(y)dy = 0.$$

Treat q_2 and q_3 similarly.

The second thing that Eq. (A1) implies is that

$$\alpha = -\int_{\mathbb{R}^3} \sum \frac{x_i - y_i}{|x-y|^3} *p\tau_i - \int_{\mathbb{R}^3} \sum_{ij} \frac{x_i - y_i}{|x-y|^3} \tau_i q_j \tau_j.$$

Using again the multipole expansion

$$\frac{x_i - y_i}{|x-y|^3} = \frac{x_i}{|x|^3} - \frac{y_i}{|x|^3} + \cdots = \frac{x_i}{|x|^3} + O(|x|^{-3})$$

and the fact that the decay conditions on p and q give bounded integrals,

$$\alpha = -\sum_i \frac{x_i}{|x|^3} \int_{\mathbb{R}^3} *p\tau_i + \frac{1}{|x|^3} \sum_i \int_{\mathbb{R}^3} y_i *p\tau_i + \cdots - \sum_{i\neq j} \frac{x_i}{|x|^3} \int_{\mathbb{R}^3} \tau_i q_j \tau_j + \frac{1}{|x|^3} \sum_{i\neq j} \int_{\mathbb{R}^3} y_i \tau_i q_j \tau_j + O(|x|^{-3}).$$

Finally, using that

$$\int_{\mathbb{R}^3} q_i(y)dy = 0$$

we can write, going back to the differential forms of notation:

$$\alpha = -\left(\int_{\mathbb{R}^3} *p(y)dy\right) \sum_i \frac{x_i}{|x|^3} dx_i + O(|x|^{-3}).$$

Now notice that in polar coordinates

$$\sum_i \frac{x_i}{|x|^3} dx_i = r\,dr,$$

hence,

$$\alpha = Cr^{-2}\,dr + O(|x|^{-3}).$$

Since we had set $\alpha = \langle \Phi, *_E F_A \rangle$, we have on $\mathbb{R}^3$:

$$\langle \Phi, F_A \rangle = C \sin\theta\, d\varphi \wedge d\theta + O(|x|^{-3}).$$

Since we have not presented any formulas for the magnetic charge of a monopole solution, we do it here. Notice that by definition

$$C = \int_{\mathbb{R}^3} *p(y)dy = \int_{\mathbb{R}^3} \langle d_A \Phi \wedge F_A \rangle.$$

Now the first Chern class of the reduced bundle over S^2 is given by

$$c_1 = \frac{1}{4\pi} \int_{S^2} \langle F_{A_\infty}, \Phi_\infty \rangle = \frac{1}{4\pi} C\,\mathrm{vol}(S^2) = C.$$

Since the reduced bundle is nothing but the pull-back bundle via Φ_∞ of the Hopf fibration $U(1) \to SU(2) \to S^2$ we have that $c_1 = \deg(\Phi_\infty)$. That is, we recover the well-known formula for magnetic charge:

$$\text{Magnetic charge} \equiv \deg(\Phi_\infty) = \int_{\mathbb{R}^3} \langle d_A \Phi \wedge F_A \rangle.$$

Or, as physicists argue, see Schwarz,[18] the magnetic field is the projection of the electromagnetic field on the Higgs direction and the magnetic charge is obtained by integrating the magnetic flux.

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Norms of Bethe wave functions for the nonlinear Schrödinger model of spin-1/2 particles

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A formula for scalar products of Bethe wave functions in the nonlinear Schrödinger model of spin-$\frac{1}{2}$ particles is proposed. It is shown, in addition, that one can replace conjugate states by dual eigenfunctions to calculate correlation functions for integrable systems.

I. INTRODUCTION AND BETHE WAVE FUNCTIONS OF THE MODEL

Recently, there has been much interest in the calculations of the correlation functions for integrable models.[1] A first step toward this goal is to calculate the norms of the Bethe wave functions.[2] Norms of the eigenfunctions for the nonlinear Schrödinger model of spin-zero particles and for the xxz Heisenberg chains were obtained before.[3,4] The main purpose of this paper is to study the norms of Bethe wave functions for the nonlinear Schrödinger model of spin-$\frac{1}{2}$ particles.

The Hamiltonian for the nonlinear Schrödinger model of spin-$\frac{1}{2}$ particles with repulsive interaction is

$$H=\int dx\left\{\frac{\partial U^{+}}{\partial x}\frac{\partial U}{\partial x}+c:U^{+}UU^{+}U:\right\}, \tag{1}$$

where $c>0$ is the coupling constant. The field operator $U=\binom{U_1}{U_2}$ has two components and they satisfy the anticommutation relations

$$\{U_i(x,t),U_j^{+}(x',t)\}=\delta_{ij}\delta(x-x'),$$
$$\{U_i(x,t),U_j(x',t)\}=0,\quad i,j=1,2. \tag{2}$$

Note that H has been diagonalized by QISM in Ref. 5. The associated monodromy matrix (on lattice interval $[0,L]$)

$$T_L(\lambda)=\begin{pmatrix}A_{11}(\lambda) & A_{12}(\lambda) & B_1(\lambda)\\ A_{21}(\lambda) & A_{22}(\lambda) & B_2(\lambda)\\ C_1(\lambda) & C_2(\lambda) & D(\lambda)\end{pmatrix}\equiv\begin{pmatrix}A(\lambda) & B(\lambda)\\ C(\lambda) & D(\lambda)\end{pmatrix} \tag{3}$$

is a 3×3 matrix in the present case. Commutation relations between these matrix elements are given by formula

$$T_{ki}(\lambda)T_{lj}(\mu)=T_{lj}(\mu)T_{ki}(\lambda)(-1)^{[p(k)+p(i)][p(l)+p(j)]}+\frac{b(\lambda-\mu)}{a(\lambda-\mu)}(-1)^{p(l)p(k)+p(i)p(l)+p(k)p(i)}[T_{li}(\mu)\times T_{kj}(\lambda)-T_{li}(\lambda)T_{kj}(\mu)],\quad i,j,k,l=1,2,3, \tag{4}$$

where

$$p(i)=\begin{cases}0, & \text{when } i=1,2,\\ 1, & \text{when } i=3,\end{cases}$$
$$a(\lambda)=1-b(\lambda)=\lambda/(\lambda+ic). \tag{5}$$

The Hamiltonian H and the transfer matrix str $T_L(\lambda)\equiv A_{11}(\lambda)+A_{22}(\lambda)-D(\lambda)$ have common eigenfunctions that are constructed by

$$|\psi(u_1\cdots u_n;\{v_i\})\rangle=C(u_1)\otimes\cdots\otimes C(u_n)|o\rangle\times C^{(1)}(v_1)\cdots C^{(1)}(v_m)|o^{(1)}\rangle, \tag{6}$$

provided that $\{u_i\}$ and $\{v_i\}$ satisfy the following Bethe ansatz equations:

$$\frac{\tilde{a}(u_l)}{\tilde{d}(u_l)}=\prod_{i=1}^{m}a(v_i-u_l),\quad l=1,\ldots,n,$$
$$\prod_{l=1}^{n}a(v_i-u_l)=\prod_{\substack{j=1\\ j\neq i}}^{m}\left\{\frac{a(v_i-v_j)}{a(v_j-v_i)}\right\},\quad i=1,\ldots m, \tag{7}$$

where $|o\rangle$ is the pseudovacuum and

$$A(\lambda)|o\rangle=\begin{pmatrix}\tilde{a}(\lambda) & 0\\ 0 & \tilde{a}(\lambda)\end{pmatrix}|o\rangle,$$
$$D(\lambda)|o\rangle=\tilde{d}(\lambda)|o\rangle,\quad B(\lambda)|o\rangle=0. \tag{8}$$

Here, $C^{(1)}(v)$ is an element of matrix $T^{(1)}(v)$, which is defined by

$$T^{(1)}(v)=\begin{pmatrix}A^{(1)}(v) & B^{(1)}(v)\\ C^{(1)}(v) & D^{(1)}(v)\end{pmatrix}=L_n(v-u_n)\cdots L_1(v-u_1), \tag{9}$$

where

$$L_j(v)=a(v)\sum_{a,b=1}^{2}e^{aa}\otimes e_j^{bb}+b(v)\sum_{a,b=1}^{2}e^{ab}\otimes e_j^{ba} \tag{10}$$

can be considered[5] as the transfer matrix at site j of a Heisenberg ferromagnetic chain with dynamical variables e_j^{ab}, and the associated vacuum $|o^{(1)}\rangle$ is defined by

$$|o^{(1)}\rangle=\begin{pmatrix}0\\ 1\end{pmatrix}_1\otimes\cdots\otimes\begin{pmatrix}0\\ 1\end{pmatrix}_n. \tag{11}$$

The Yang–Baxter relation for $L_j(v)$ is

$$r(v_1-v_2)[L_j(v_1)\otimes L_j(v_2)]=[L_j(v_2)\otimes L_j(v_1)]r(v_1-v_2), \tag{12}$$

where

$$r(v)\equiv b(v)+a(v)\sum_{i,j=1}^{2}e^{ij}\otimes e^{ji} \tag{13}$$

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and e^{ij} is in a two-dimensional auxiliary space.

The eigenvalue of H is given by

$$E(c)=\frac{\langle\psi(u_1\cdots u_n;\{v_i\})|H|\psi(u_1\cdots u_n;\{v_i\})\rangle}{\langle\psi(u_1\cdots u_n;\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle}$$
$$=\sum_{i=1}^{n}u_i{}^2. \tag{14}$$

It can be shown that

$$\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|$$
$$\equiv\langle o^{(1)}|\tilde{B}^{(1)}(v_m)\cdots\tilde{B}^{(1)}(v_1)\langle o|B(u_n)$$
$$\otimes\cdots\otimes B(u_1) \tag{15}$$

is the dual eigenfunction of str $T_L(\lambda)$ with the same eigenvalue as $|\psi(u_1\cdots u_n;\{v_i\})\rangle$, which is to say

$$\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\text{str}\,T_L(\lambda)$$
$$=\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\theta(\lambda,\{u_i\},\{v_i\}), \tag{16}$$

where $\theta(\lambda,\{u_i\},\{v_i\})$ also satisfies

$$\text{str}\,T_L(\lambda)|\psi(u_1\cdots u_n;\{v_i\})\rangle$$
$$=\theta(\lambda,\{u_i\},\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle. \tag{17}$$

The operator $\tilde{B}^{(1)}(v)$ in (15) is defined by

$$\tilde{B}^{(1)}(v)\equiv(1,0)\{L_n(v-u_1)\cdots L_1(v-u_n)\}\begin{pmatrix}0\\1\end{pmatrix}. \tag{18}$$

If we write

$$C^{(1)}(v_1)\cdots C^{(1)}(v_m)|o^{(1)}\rangle$$
$$\equiv\sum_{\{\alpha_i\}}g_{\alpha_1\cdots\alpha_n}(u_n\cdots u_1)(\alpha_1)_1\otimes\cdots\otimes(\alpha_n)_n,$$
$$\langle o^{(1)}|\tilde{B}^{(1)}(v_m)\cdots\tilde{B}^{(1)}(v_1)$$
$$\equiv\sum_{\{\alpha_i\}}\tilde{g}'_{\alpha_1\cdots\alpha_n}(u_1\cdots u_n)(\alpha_1)_1{}^{+}\otimes\cdots\otimes(\alpha_n)_n{}^{+}, \tag{19}$$

where $(\alpha_i)_i=\binom{0}{1}_i$ or $\binom{1}{0}_i$, then we can also show that (see Appendix A)

$$g_{\alpha_1\cdots\alpha_l\alpha_{l+1}\cdots\alpha_n}(u_n\cdots u_{l+1}u_l\cdots u_1)$$
$$=\frac{1}{a(u_l-u_{l+1})}\{g_{\alpha_1\cdots\alpha_{l+1}\alpha_l\cdots\alpha_n}(u_n\cdots u_lu_{l+1}\cdots u_1)$$
$$-b(u_l-u_{l+1})g_{\alpha_1\cdots\alpha_{l+1}\alpha_l\cdots\alpha_n}(u_n\cdots u_{l+1}u_l\cdots u_1)\}. \tag{20}$$

II. NORMS OF THE BETHE WAVE FUNCTIONS

In physics, the correlation function in state $|\psi\rangle$ is generally expressed by $\langle\psi|P|\psi\rangle/\langle\psi|\psi\rangle$, where $\langle\psi|=|\psi\rangle^{+}$ and P is an operator. The first step to calculate this correlation function is to calculate the norm $\langle\psi|\psi\rangle$.[2] However, it is almost impossible in the present problem to calculate $\langle\psi|\psi\rangle$ directly from the Yang–Baxter relation between $T_L{}^{+}(u)$ and $T_L(v)$ even in the simplest case, e.g., $\langle o|C_1{}^{+}(u)C_1(u)|o\rangle$. Therefore, an attempt to replace $\langle\psi|$ by the dual eigenfunction $\langle\tilde{\varphi}|$ arose. Since

$$C(u)\neq B^{+}(u),\quad \tilde{B}^{(1)}(u)\neq[C^{(1)}(u)]^{+} \tag{21}$$

in our problem, the conjugate state $\langle\psi|$ is generally not equal to the dual eigenfunction $\langle\tilde{\varphi}|$. However, it can be shown that for integrable systems we have (see Appendix B)

$$\langle\psi|P|\psi\rangle/\langle\psi|\psi\rangle=\langle\tilde{\varphi}|P|\psi\rangle/\langle\tilde{\varphi}|\psi\rangle. \tag{22}$$

So we can replace $\langle\psi|$ by $\langle\tilde{\varphi}|$ to calculate the correlation function, and the remaining part of this paper is devoted to proposing a formula for the scalar product between $|\psi\rangle$ and the dual eigenfunction $\langle\tilde{\varphi}|$, which is proportional to the norm $\langle\psi|\psi\rangle$, as shown in Appendix B.

For some small values of m and n, one can see by direct calculation that $\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle$ is proportional to

$$D_{n,m}\equiv\det_n\left\{\frac{\bar{\partial}\varphi_k{}^0}{\bar{\partial}u_l}\right\}\det_m\left\{\frac{\partial\varphi_j{}^1}{\partial v_i}\right\}, \tag{23}$$

which is the denominator in the expression of $\partial u_i/\partial c$ obtained from (7) by differentiating the logarithm and the Jacobi matrixes[4] in (23) are defined by

$$\frac{\bar{\partial}\varphi_k{}^0}{\bar{\partial}u_l}\equiv\frac{\partial\varphi_k{}^0}{\partial u_l}-\sum_{\alpha,\beta=1}^{m}\left(\frac{\partial\varphi_k{}^0}{\partial v_\beta}\right)(M^{-1})_{\beta\alpha}\left(\frac{\partial\varphi_\alpha{}^1}{\partial u_l}\right),$$
$$\varphi_k{}^0\equiv\ln\left(\frac{\tilde{a}(u_k)}{\tilde{d}(u_k)}\right)+\sum_{j=1}^{m}\ln\left(\frac{1}{a(v_j-u_k)}\right),$$
$$M\equiv\left\{\frac{\partial\varphi_j{}^1}{\partial v_i}\right\}_{m\times m},$$
$$\varphi_j{}^1\equiv\sum_{i=1}^{n}\ln a(v_j-u_i)+\sum_{\substack{k=1\\k\neq j}}^{m}\ln\left(\frac{a(v_k-v_j)}{a(v_j-v_k)}\right). \tag{24}$$

Comparing the present case with that of spin-zero, we conjecture, leaving its justification to be discussed in later publications, that the proportional relation between $\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle$ and $D_{n,m}$ is valid, in general, and we write

$$\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle=fD_{n,m}, \tag{25}$$

the coefficient f is determined in the following.

Now we consider

$$I\equiv\langle o^{(1)}|\tilde{B}^{(1)}(v_m)\cdots\tilde{B}^{(1)}(v_1)\langle o|B(u_n{}^B)\otimes\cdots\otimes B(u_1{}^B)C(u_1{}^C)\otimes\cdots\otimes C(u_n{}^C)|o\rangle C^{(1)}(v_1)\cdots C^{(1)}(v_m)|o^{(1)}\rangle$$
$$=\sum_{\{\alpha_i\alpha_i'\}}\{\tilde{g}'_{\alpha_1'\cdots\alpha_n'}(u_1{}^B\cdots u_n{}^B)g_{\alpha_1\cdots\alpha_n}(u_n{}^C\cdots u_1{}^C)\langle o|B_{\alpha_1'}(u_n{}^B)\cdots B_{\alpha_n'}(u_1{}^B)C_{\alpha_1}(u_1{}^C)\cdots C_{\alpha_n}(u_n{}^C)|o\rangle\}$$
$$\equiv\sum_{\{\alpha_i\alpha_i'\}}\{\tilde{g}'_{\alpha_1'\cdots\alpha_n'}(u_1{}^B\cdots u_n{}^B)g_{\alpha_1\cdots\alpha_n}(u_n{}^C\cdots u_1{}^C)I_1\}, \tag{26}$$

where $u_i{}^C(u_i{}^B)$ is different from $u_j{}^C(u_j{}^B)$ when $i\neq j$.

It is easily seen that

$$\langle\tilde{\varphi}(u_n\cdots u_1;\{v_i\})|\psi(u_1\cdots u_n;\{v_i\})\rangle=I|_{u_i{}^C=u_i{}^B}, \tag{27}$$

which may be calculated from (26) by using (4) and (8) after taking limit $u_i{}^C\to u_i{}^B$.

From (4) and (8), we see that I_1 is a function of

$a^{-1}(u_i^{B(C)} - u_{j\neq i}^{B(C)})$, $a^{-1}(u_i^{B(C)} - u_j^{C(B)})$,

$\tilde{a}(u_i^{B(C)})$, and $\tilde{d}(u_i^{B(C)})$. Thus I_1 has poles in the limit $u_i^C \to u_i^B$ due to the factor $a^{-1}(u_i^{B(C)} - u_i^{C(B)})$. When we use l'Hopital's rule to calculate the resides, we will find that there are terms proportional to $x_i \equiv \partial \ln[\tilde{a}(u_i)/\tilde{d}(u_i)]/\partial u_i$, which can be considered as a variable independent of $\{u_j\}$ according to the discussing in Ref. 4. The interesting term in I after taking limit $u_i^C \to u_i^B$ is the term proportional to $\Pi_{i=1}^n x_i$, which can be easily calculated by using (4), (8), and (20), and the result is (here we have set $\langle o|o\rangle = 1$)

$$I|_{u_i^B = u_i^C} = (-ic)^n \left\{ \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} \left(\frac{1}{a(u_i - u_j)} \right)^2 \right\} \times \left[\prod_{i=1}^{n} \tilde{a}(u_i)\tilde{d}(u_i) \right] \times \left[\sum_{\{\beta_i\}} \tilde{g}'_{\beta_n \cdots \beta_1}(u_1 \cdots u_n) g_{\beta_n \cdots \beta_1}(u_1 \cdots u_n) \right] \times \left[\prod_{i=1}^{n} x_i \right] + Q, \tag{28}$$

where Q is a polynomial and each term of Q does not depend on all x_i, $i = 1,...,n$.

Since

$$I_2 \equiv \sum_{\{\beta_i\}} \tilde{g}'_{\beta_n \cdots \beta_1}(u_1 \cdots u_n) g_{\beta_n \cdots \beta_1}(u_1 \cdots u_n) = \langle o^{(1)}|\tilde{B}^{(1)}(v_m) \cdots \tilde{B}^{(1)}(v_1)\tilde{C}^{(1)}(v_1) \cdots \times \tilde{C}^{(1)}(v_m)|o^{(1)}\rangle, \tag{29}$$

where

$$\tilde{C}^{(1)}(v) \equiv (0,1)\{L_n(v - u_1) \cdots L_1(v - u_n)\}\begin{pmatrix}1\\0\end{pmatrix}, \tag{30}$$

and the Yang–Baxter equation (12) for $L_j(v)$ is similar to that for the xxx model, we can use Korepin's result[4] to calculate I_2, and the obtained result is

$$I_2 = (ic)^m \left[\prod_{j=1}^{m} \prod_{\substack{k=1 \\ \neq j}}^{m} \frac{1}{a(v_j - v_k)} \right] \det_m \left\{ \frac{\partial \varphi_k^{\,1}}{\partial v_j} \right\}. \tag{31}$$

Substitute (31) into (28) and comparing it to (25), we now obtain

$$f = (-ic)^n \left\{ \prod_{i=1}^{n-1} \prod_{j=i+1}^{n} \left[\frac{1}{a(u_i - u_j)} \right]^2 \right\} \times \left[\prod_{i=1}^{n} \tilde{a}(u_i)\tilde{d}(u_i) \right] (ic)^m \left[\prod_{j=1}^{m} \prod_{\substack{k=1 \\ \neq j}}^{m} \frac{1}{a(v_j - v_k)} \right] \times \left[\prod_{i=1}^{n} \tilde{a}(u_i)\tilde{d}(u_i) \right] \det_n \left\{ \frac{\bar{\partial} \varphi_k^{\,0}}{\bar{\partial} u_l} \right\} (ic)^m \times \left[\prod_{j=1}^{m} \prod_{\substack{i=1 \\ \neq j}}^{m} \frac{1}{a(v_j - v_i)} \right] \det_m \left\{ \frac{\partial \varphi_k^{\,1}}{\partial v_l} \right\}, \tag{33}$$

where the Jacobi matrices are defined by (24). We have explicitly verified (33) by direct calculation for some small values of m and n, e.g., $n = 2$ and $m = 1$. A proof of the formula (33) for arbitrary n and m is needed.

APPENDIX A: PROPERTIES OF $g_{\alpha_1 \cdots \alpha_n}(u_n \cdots u_1)$

From definition (19), we have

$$g_{\alpha_1 \cdots \alpha_n}(u_n \cdots u_1) = (\alpha_1)_1^+ \otimes \cdots \otimes (\alpha_n)_n^+ \times C^{(1)}(v_1) \cdots C^{(1)}(v_m)|o^{(1)}\rangle. \tag{A1}$$

Now we write

$$(\alpha_1)_1^+ \otimes \cdots \otimes (\alpha_n)_n^+ \equiv \prod_{j=1}^{n} \alpha_j^+$$

$$|o^{(1)}\rangle = \begin{pmatrix}0\\1\end{pmatrix}_1 \otimes \cdots \otimes \begin{pmatrix}0\\1\end{pmatrix}_n \equiv \prod_{i=1}^{n} \downarrow_i,$$

$$C^{(1)}(v_\beta) = (0,1)\{L_n(v_\beta - u_n) \cdots L_1(v_\beta - u_1)\}\begin{pmatrix}1\\0\end{pmatrix} \equiv \downarrow_\beta^+ \{L_n(v_\beta - u_n) \cdots L_1(v_\beta - u_1)\} \uparrow_\beta, \tag{A2}$$

then

$$g_{\alpha_1 \cdots \alpha_n}(u_n \cdots u_1) = \left\{ \prod_{j=1}^{n} \alpha_j^+ \right\} \left\{ \prod_{\beta=1}^{m} \downarrow_\beta^+ [L_n(v_\beta - u_n) \cdots L_1(v_\beta - u_1)] \uparrow_\beta \right\} \left\{ \prod_{i=1}^{n} \downarrow_i \right\} = \left\{ \prod_{\beta=1}^{m} \downarrow_\beta^+ \right\} \left\{ \prod_{j=n}^{1} \alpha_j^+ \tau(u_j) \downarrow_j \right\} \left\{ \prod_{\beta=1}^{m} \uparrow_\beta \right\}, \tag{A3}$$

$$\tau(u_j) \equiv L_j(v_1 - u_j) \cdots L_j(v_m - u_j) \equiv \begin{pmatrix} A^{(2)}(u_j) & B^{(2)}(u_j) \\ C^{(2)}(u_j) & D^{(2)}(u_j) \end{pmatrix}. \tag{A4}$$

Here we have used the fact that $L_j(v_\alpha - u_j)$ and $L_i(v_\beta - u_i)$ commutes when $\alpha \neq \beta$ and $j \neq i$. The Yang–Baxter relation for $\tau(u)$ is

$$r(u_1 - u_2)[\tau(u_2) \otimes \tau(u_1)] = [\tau(u_1) \otimes \tau(u_2)] r(u_1 - u_2). \tag{A5}$$

Since

$$g_{\alpha_1 \cdots \alpha_l \alpha_{l+1} \cdots \alpha_n}(u_n \cdots u_{l+1} u_l \cdots u_1) \sim \alpha_{l+1}^+ \tau(u_{l+1}) \downarrow_{l+1} \alpha_l^+ \tau(u_l) \downarrow_l. = (\alpha_{l+1})_{l+1}^+ \tau(u_{l+1}) \downarrow_{l+1} (\alpha_l)_l^+ \tau(u_l) \downarrow_l, \tag{A6}$$

we see from (A5) the following.

(a) When $\alpha_{l+1} = \alpha_l = \uparrow$ or $\downarrow$, we have

$$(\alpha_{l+1})_{l+1}^+ \tau(u_{l+1}) \downarrow_{l+1} (\alpha_l)_l^+ \tau(u_l) \downarrow_l = (\alpha_l)_{l+1}^+ \tau(u_l) \downarrow_{l+1} (\alpha_{l+1})_l^+ \tau(u_{l+1}) \downarrow_l = (\alpha_{l+1})_{l+1}^+ \tau(u_l) \downarrow_{l+1} (\alpha_l)_l^+ \tau(u_{l+1}) \downarrow_l. \tag{A7}$$

(b) When $\alpha_{l+1}=\uparrow$ and $\alpha_l=\downarrow$, we have

$$
\begin{aligned}
&(\alpha_{l+1})^{+}_{l+1}\tau(u_{l+1})\downarrow_{l+1}(\alpha_l)_l{}^{+}\tau(u_l)\downarrow_l \\
&\quad=B^{(2)}(u_{l+1})D^{(2)}(u_l)=[1/a(u_l-u_{l+1})]D^{(2)}(u_l)B^{(2)}(u_{l+1}) \\
&\qquad-[b(u_l-u_{l+1})/a(u_l-u_{l+1})]D^{(2)}(u_{l+1})B^{(2)}(u_l) \\
&\quad=[1/a(u_l-u_{l+1})](\alpha_l)^{+}_{l+1}\tau(u_l)\downarrow_{l+1}(\alpha_{l+1})_l{}^{+} \\
&\qquad\times\tau(u_{l+1})\downarrow_l-[b(u_l-u_{l+1})/a(u_l-u_{l+1})]\{(\alpha_l)^{+}_{l+1}\tau(u_{l+1})\downarrow_{l+1}(\alpha_{l+1})_l{}^{+}\tau(u_l)\downarrow_l\}. \qquad \text{(A8)}
\end{aligned}
$$

(c) When $\alpha_{l+1}=\downarrow$ and $\alpha_l=\uparrow$, the result is similar to that of (b). From (a)–(c), we conclude that

$$
\begin{aligned}
&g_{\alpha_1\cdots\alpha_l\alpha_{l+1}\cdots\alpha_n}(u_n\cdots u_{l+1}u_l\cdots u_1) \\
&\quad=\frac{1}{a(u_l-u_{l+1})}g_{\alpha_1\cdots\alpha_{l+1}\alpha_l\cdots\alpha_n}(u_n\cdots u_lu_{l+1}\cdots u_1) \\
&\qquad-\frac{b(u_l-u_{l+1})}{a(u_l-u_{l+1})}g_{\alpha_1\cdots\alpha_{l+1}\alpha_l\cdots\alpha_n}(u_n\cdots u_{l+1}u_l\cdots u_1). \qquad \text{(A9)}
\end{aligned}
$$

APPENDIX B: RELATION BETWEEN $\langle\tilde{\varphi}|$ AND $\langle\psi|$

Consider an integrable circular chain with the number of total degrees of freedom N. Denote $|\psi_j\rangle$ the jth eigenfunction of str $T_L(\lambda)$, $\langle\tilde{\varphi}_j|$ the jth dual eigenfunction of str $T_L(\lambda)$ with the same eigenvalue as $|\psi_j\rangle$ and $\langle\psi_j|$ the conjugate state ($|\langle\psi_j|=|\psi_j\rangle^{+}$), where $T_L(\lambda)$ is the associated monodromy matrix. Since the number of total conservative quantities is equal to the number of total degrees of freedom for intagrable systems, we assume $\{\hat{h}_\beta,\beta=1,\ldots,N\}$ are the N operators of the total conservative quantities of the integrable chain. For physics system we have $\hat{h}_i=\hat{h}_i{}^{+}$. From QISM, we know that $|\psi_j\rangle$ is the common eigenfunction of str $T_L(\lambda)$ and $\hat{h}_\beta$ for any β, and we write

$$\hat{h}_\beta|\psi_j\rangle=h_{\beta j}|\psi_j\rangle,\quad \beta=1,\ldots,N. \qquad \text{(B1)}$$

It can be shown that

$$
\begin{aligned}
&\langle\psi_j|\hat{h}_\beta=\langle\psi_j|h^{*}_{\beta j}=\langle\psi_j|h_{\beta j}, \\
&\langle\tilde{\varphi}_j|\hat{h}_\beta=\langle\tilde{\varphi}_j|h_{\beta j}, \qquad \text{(B2)}
\end{aligned}
$$

from the definition of $\langle\psi_j|$ and $\langle\tilde{\varphi}_j|$.

Since str $T_L(\lambda)$ can, and only can, generate N independent conservative quantities, there at least exists one operator, for example, $\hat{h}_\alpha$ for which $h_{\alpha i}$ is not equal to $h_{\alpha j}$ in (B1) when $i\neq j$, where $i\neq j$ means that $|\psi_i\rangle$ and $|\psi_j\rangle$ are two different eigenfunctions of str $T_L(\lambda)$, and we get

$$\langle\tilde{\varphi}_j|\psi_i\rangle=0 \text{ and } \langle\psi_j|\psi_i\rangle=0,\quad \text{when } i\neq j. \qquad \text{(B3)}$$

If we write

$$\langle\psi_j|=\sum_i f_{ji}\langle\tilde{\varphi}_i|, \qquad \text{(B4)}$$

then from (B3) we have

$$f_{ij}=\delta_{ij}\langle\tilde{\varphi}_j|\psi_j\rangle/\langle\psi_j|\psi_j\rangle. \qquad \text{(B5)}$$

Therefore,

$$\langle\psi_j|=f_{jj}\langle\tilde{\varphi}_j| \qquad \text{(B6)}$$

and

$$\langle\psi_j|P|\psi_j\rangle/\langle\psi_j|\psi_j\rangle=\langle\tilde{\varphi}_j|P|\psi_j\rangle/\langle\tilde{\varphi}_j|\psi_j\rangle, \qquad \text{(B7)}$$

where P is an arbitrary operator.

For the continuous (integrable) field-theoretical models, which have infinite number of freedom degrees, we first take their lattice forms (with N finite) and then let the lattice spacing $\Delta\to 0(N\to\infty)$. It is reasonable to conjecture that (B7) is still correct in the continuous limit $\Delta\to 0(N\to\infty)$.

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A multivectorial Dirac equation

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The multivectorial generalization of the Cartan map, for $\mathscr{C}(1,3)$ space-time Clifford algebra and an arbitrary gauge group in an isotopic space, is applied to the standard Dirac equation to generate the multivectorial Dirac equation. Using both geometrical and physical reasoning, a particular case discussed by Reifler and Morris [J. Math. Phys. **26**, 2059 (1985)] is projected from the general multivectorial Dirac equation, to discuss the properties and limitations associated to their quaternion model. The use of the general multivectorial Dirac equation, which can be defined on any space-time manifold, is also illustrated.

I. INTRODUCTION

Historically the dynamical equations for particles and fields have been developed using several mathematical structures including tensors, spinors, and twistors. However, spinor fields can only be defined on a restricted class of manifolds admitting spin structure.[1-3] Therefore it is desirable to show the relations between these structures to overcome as many limitations as possible in a physical model.

On the other hand, multivectorial fields can be defined on any manifold[4-6] (parallelizable or not) and they include all the previous mathematical structures in an unified language. We constructed a multivectorial generalization of the Cartan map,[7] mapping Weyl spinors into complex quaternions, to a mapping from any dimensional spinor spaces (we used the concept of spinor-like minimum ideal of a nondegenerate Clifford algebra) onto a multivectorial space with two symmetries, one of them being the space-time Clifford group $\mathscr{C}(1,3)$ and another one being an isotopic space group (in multivectorial representation) related with the most common gauge groups in quantum field theory. The algebraic properties of this map and of the operators representing observables studied previously[7] will be used in this paper. We will apply this multivectorial Cartan map to the Dirac equation to obtain the multivectorial Dirac equation, that is, one where the field representing the particle is a multivector [in $\mathscr{C}(1,3)$ space-time and a chosen gauge group], obtained through the application of the multivectorial Cartan map to the original Dirac spinor. The method is general and can be used for other formalism or equations.

The present paper should also illustrate how it is possible to obtain dynamical equations for fields, fermionic or bosonic, within one common mathematical structure, namely the Clifford algebra.

Section II describes the multivectorial generalization of the Cartan map and its use to obtain a multivectorial form of the Dirac's equation. Section III discusses the particular case where the general multivectorial Dirac equation is projected onto its complex quaternionic part with SU(2) gauge group in the isotopic space. Finally, we will present some particular remarks about useful applications and properties related to elementary particles theories.

II. THE APPLICATION OF THE MULTIVECTORIAL CARTAN MAP TO THE DIRAC EQUATION

It is possible to write the Dirac equation for a massive particle as the following system of equations:[8,9]

$$\begin{aligned} &i(\hat{\sigma}_0 D^0 + \hat{\sigma}_i D^i)\bar{\eta} = m_0 \zeta, \\ &i(\hat{\sigma}_0 D^0 - \hat{\sigma}_i D^i)\zeta = m_0 \bar{\eta}, \end{aligned} \tag{2.1}$$

considering the Dirac bispinor $\psi = (\zeta, \bar{\eta})$ (in chiral representation) as a composite object, consisting of one Weyl spinor $\xi \in C^2$ and a conjugate Weyl spinor $\bar{\eta} \in C^2$; where if

$$\eta = \begin{pmatrix} \eta_1 \\ \eta_2 \end{pmatrix} \text{ then } \bar{\eta} = \begin{pmatrix} -\eta_2^* \\ \eta_1^* \end{pmatrix},$$

$$\hat{\sigma}_\alpha = (\mathbf{1}, \sigma_{\text{Pauli}}), \quad \alpha = 0,1,2,3;$$

$(D^0, D^i); i = 1,2,3$, are the components of the quadrimoment operator and m_0 is the rest mass associated to ψ (η_i^* is the usual complex conjugate of the complex number η_i) and the summation convention is used.

Following Reifler[5] we combine the system (2.1) in the following way:

$$i\sigma_\alpha D^\alpha \psi = -\phi^\alpha \tau_\alpha \bar{\psi} \tag{2.2}$$

where now the $\sigma_\alpha = (\mathbf{1} \otimes \hat{\sigma}_0, -\mathbf{1} \otimes \hat{\sigma}_i)$ are 4×4 matrices representing the scalar and the bivectors $e_0 e_i$ of space-time, $\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$ is a Dirac spinor pair, $\bar{\psi}$ is its spinor conjugate given by $\bar{\psi} = \begin{pmatrix} -\bar{\eta} \\ \bar{\xi} \end{pmatrix}$, $\phi^\alpha = (0,0,0,m)$ is a mass quaternion,[5,6] and the 4×4 matrices $\tau_\alpha = (\mathbf{1}, \tau_i)$ connect the SU(2) generators of the "isotopic" space, $\tau_i = \hat{\tau}_i \otimes \mathbf{1}$.

In Eq. (2.2) the ϕ^α term chooses the τ_α generator in such a way that the Dirac mass can be defined through a mixing of the left and right chiralities in the correct proportion.

The original Cartan map[10] is a map $M(\eta,\eta'): C^2 \times C^2 \to \mathscr{C}(3,0)$ of Weyl spinors into the complex quaternions. Here we will use the multivectorial generalization of the Cartan map $M_\omega(\psi,\psi'): C^4 \times C^4 \to \mathscr{C}(1,3)$ given by

$$M_\omega(\psi,\psi') = M_\omega^\alpha(\psi,\psi')\Gamma_\alpha, \tag{2.3a}$$

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which, if $\psi^T\Gamma_\alpha\lambda_\omega^*\epsilon\psi' = \lambda_\omega\psi^T\Gamma_\alpha\epsilon\psi'$ (this is an important result of the generalized Cartan map[7]), is equivalent for all β to

$$M_\omega(\psi,\psi') = 4\lambda_\omega\tau_3(\epsilon\psi'\psi^T)^T\tau_3. \tag{2.3b}$$

In this expression:

(i) $\psi,\psi'\in C^4$ are minimum left ideals of $C(1,3)$[1,2,3,11] (this is the Clifford group associated with the $A_{1,3}$ space-time[12-14]) and ϵ is a spinor metric

$$\epsilon = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

such that the $\bar{\bar{\psi}} = \psi$ bijection is true. ψ^T is the ψ spinor transpose.

(ii) $\Gamma_\alpha\in\mathscr{C}(1,3)$ with $\alpha = 0,\ldots,15$ is a 4×4 representation of a basis set for the multivectors of space-time.[12,13]

(iii) λ_ω is the multivectorial representation for a given Lie group used as a gauge group.[14]

(iv) $\tau_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ is a 4×4 supermatrix, the **1** are 2×2 unit matrices, denoting here a SU(2) *isotopic* direction.

(v) The components of the multivectorial Cartan map are

$$M^\alpha_\beta(\psi,\psi') = \psi^T\Gamma^\alpha(\lambda_\omega\bar{\psi}')^* = \psi^T\Gamma^\alpha\lambda_\omega^*\epsilon\psi',$$

given that $\bar{\psi}'^* = \epsilon\psi'$.

Using (2.3) in the Dirac equation (2.2) we obtain

$$iM_\omega(\psi,\sigma_\alpha D^\alpha\psi) = -M_\omega(\psi,\phi^\beta\tau_\beta\bar{\psi}) \tag{2.4}$$

but as $\lambda_0 = 1$ then

$$iM_0(\psi,\sigma_\alpha D^\alpha\psi) = 4\tau_3(\epsilon D^\alpha\sigma_\alpha\psi\psi^T)^T\tau_3 \tag{2.5a}$$

from (2.3b) above and we can develop the quantity in parenthesis, simplifying

$$\begin{aligned} iM_0(\psi,&D^\alpha\sigma_\alpha\psi) \\ &= \tfrac{1}{2}[\tau^0D^0M_0(\psi,\psi)\sigma_0 + \tau^1D^1M_1(\psi,\psi)\sigma_1 \\ &\quad + \tau^2D^2M_2(\psi,\psi)\sigma_2 + \tau^3D^3M_3(\psi,\psi)\sigma_3] \\ &= \tfrac{1}{2}\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta}, \end{aligned} \tag{2.5b}$$

$$\delta^{\alpha'\beta'}_{\alpha\beta} = \begin{cases} 1, & \text{if } \alpha=\alpha'=\beta=\beta' \\ & (\text{with } \alpha,\alpha',\beta,\beta' = 0,1,2,3) \\ 0, & \text{otherwise,} \end{cases}$$

where the differential operator acts on the multivector field $M_\alpha(\psi,\psi)$. The prefactors of the M_α satisfy the following relation [from (2.3b)] $M_\omega(\psi,\psi') = \lambda_\omega M_0(\psi,\psi')$, the λ_ω are matrices belonging to the chosen Lie gauge group.

The right-hand side of (2.4) is such that

$$M_0(\psi,\phi^\alpha\tau_\alpha\bar{\psi}) = 4\tau_3(\epsilon\phi^\alpha\tau_\alpha\bar{\psi}\psi^T)^T\tau_3 \tag{2.6}$$

is equivalent to

$$\begin{aligned} M_0(\psi,&\phi^\alpha\tau_\alpha\bar{\psi}) \\ &= \phi^0M_0(\psi,\bar{\psi}) + \phi^1M_0(\psi,\bar{\psi})\tau_1 + \phi^2M_0(\psi,\bar{\psi})\tau_2 \\ &\quad + \phi^3M_0(\psi,\bar{\psi})\tau_3 \\ &= M_0(\psi,\bar{\psi})\phi^\alpha\tau_\alpha, \end{aligned}$$

then

$$M_\omega(\psi,\phi^\alpha\tau_\alpha\bar{\psi}) = \lambda_\omega M_0(\psi,\bar{\psi})\phi^\alpha\tau_\alpha$$

to obtain

$$M_\omega(\psi,\phi^\alpha\tau_\alpha\bar{\psi}) = M_\omega(\psi,\bar{\psi})\phi^\alpha\tau_\alpha. \tag{2.7}$$

Consequently, the set of multivector Dirac equations (under a λ_ω gauge group in isotopic space) can be written as

$$(\lambda_\omega/2)\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} = -M_\omega(\psi,\bar{\psi})\phi^\alpha\tau_\alpha, \tag{2.8}$$

in fact (2.8) defines a system of Dirac equations for each of the λ_ω isotopic directions of the gauge group chosen in an isotopic space,. If $\omega = 0$ or $\lambda_\omega = 1$ then (2.8) reduces to

$$\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} = -2M_0(\psi,\bar{\psi})\phi^\alpha\tau_\alpha, \tag{2.9}$$

the reference multivectorial Dirac equation.

We introduced in a recent[15] paper the geometrical interpretation of the generalized, Fierz identities as the Clifford product of multivectorial Cartan maps

$$M_i(\psi,\chi)M_j(\chi',\psi') = 4M_j(\psi,\psi')M_i(\chi',\chi), \tag{2.10}$$

where the elements of the minimum ideals of the multivector algebra are $\chi,\psi,\chi',\psi'\in C^4$ and $M_i(\psi,\chi)\in C(1,3)$, $M_j(\psi,\psi') = \cdot\psi^T\lambda_j'\epsilon\psi'$, with $\lambda_j' = \tau_3\lambda_j^T\tau_3$. Finally $M_i(\psi,\chi)$ and $M_j(\psi,\chi)$ belong to a chosen Lie group algebra.

This can be used to transform the sets of equations (2.8) thus: take a particular λ_{i_1} isotopic direction in Eq. (2.8)

$$\lambda_{i_1}\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} = -2M_{i_1}(\psi,\bar{\psi})\phi^\beta\tau_\beta,$$

and multiply this equation by $M_{i_2}(\psi,\psi)$ $(\lambda_{i_2}\neq\lambda_{i_1})$ both generators of a Lie group

$$\begin{aligned} &M_{i_2}(\psi,\psi)\lambda_{i_1}\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} \\ &\quad = -2M_{i_1}(\psi,\psi)M_i(\psi,\bar{\psi})\phi^\beta\tau_\beta. \end{aligned} \tag{2.11}$$

Using the generalized Fierz identities (2.10), then (2.11) can be written

$$\begin{aligned} &M_{i_2}(\psi,\psi)\lambda_{i_1}\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} \\ &\quad = -2M_{i_1}(\psi,\bar{\psi})\,M_{i_2}(\psi,\psi)\phi^\beta\tau_\beta. \end{aligned} \tag{2.12}$$

Repeating over all gauge group generators different from i_2, we obtain

$$\begin{aligned} &\prod_{i=i_2}^{i_n} M_i(\psi,\psi)\lambda_{i_1}\tau^\alpha D^\beta M_{\alpha'}(\psi,\psi)\sigma_\beta\delta^{\alpha'\beta'}_{\alpha\beta} \\ &\quad = -2M_{i_1}(\psi,\bar{\psi})\prod_{i=i_n}^{i_2} M_i(\psi,\psi)\phi^\beta\tau_\beta. \end{aligned} \tag{2.13}$$

Then the use of the generalized Fierz identity rotates the original multivector Dirac equation (2.8) into another (2.12) containing the same information.

III. A PARTICULAR CASE OF THE MULTIVECTOR DIRAC EQUATION

We will now obtain, guided by physical and geometrical considerations, a known particular example of the system of equations (2.8). This should illustrate the advantages obtained with the use of a multivectorial analysis.

Introducing an SU(2) gauge group and a *space-time cut* (that is a quaternion basis for space-time $\sigma_\mu = \lambda_0\lambda_\mu$, where the space-time vectors γ_μ are projected relative to a given γ_0 proper time), which singles out the temporal component of the momentum differential operator from the spatial compo-

nents, then (2.8) changes to

$$P_+\tau_i\tau^0 M_0(\psi,D^0\psi)\sigma_0 + P_-\tau_i\tau^j M_{j'}(\psi,D^K\psi)\sigma_K\delta^{j'K'}_{jK} = -M_i(\psi,\bar{\psi})\phi^\beta\tau_\beta, \tag{3.1}$$

here, $\delta^{j'K'}_{jK} = \begin{cases} 1, & \text{if } j=k=k'=j' \\ & (\text{with } j,k,j',k'=1,2,3), \\ 0, & \text{otherwise} \end{cases}$

the τ_i are SU(2) generators,

$$P_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

and D^α is the covariant differential operator applied to the arguments of the spinors.

The space-time cut allows the change [see (3.2) below] from Pauli matrices to Proca matrices [see (3.2), (ii) below] of the proper Lorentz group matrix representation for the differential operator basis. The following procedure is then followed: the left-hand side term of (3.1) will be projected on the quaternion basis (σ_0,σ_j) such that we can separate the time and space components of the differential operator. Then the generalized Fierz identities (2.10)[15] are applied to rearrange the temporal and spatial components (the new components are lineal functions of the previous ones) over the Proca representation for the differential operator basis. And, finally, the quaternion subalgebra of the multivector Cartan map is projected. Doing this the equation is changed to

$$\begin{aligned} &\tau_{\mathbf{1}}^{\pm}{}_{\mathbf{1}}\left[B^0_0(\psi,\psi)P_a + \tfrac{1}{4}B^0_\beta(\psi,\psi)\tau_j\tau^\beta\tau_j P_b\right] \\ &\quad\times\{P_+\tau_i\tau^0 M_0(D^0\psi,\psi)\sigma_0 \\ &\quad + P_-\tau_i\tau^j M_{j'}(\psi,D^K\psi)\sigma_K\delta^{j'K'}_{jK}\}\begin{pmatrix}\sigma^0\\ \sigma^j\end{pmatrix}\tau_{\mathbf{1}}^{\mp}{}_{\mathbf{1}}\begin{pmatrix}\Sigma\\ \Sigma^0_j\end{pmatrix} \\ &\quad = -\tau_{\mathbf{1}}^{\pm}{}_{\mathbf{1}}\left[(i/2)B^0_0(\psi,\psi)(\phi^\beta\tau_\beta M_i(\psi,\bar{\psi}))\right]\tau_{\mathbf{1}}^{\mp}{}_{\mathbf{1}}, \end{aligned} \tag{3.2}$$

where

(i) $\tau_{\mathbf{1}}^{\pm}{}_{\mathbf{1}}$ and $\tau_{\mathbf{1}}^{\mp}{}_{\mathbf{1}}$ denote the operators that project the quaternion part of any multivector placed between them,[7] that is, if we want to obtain the quaternion part of a given multivector A, we denote it as the sum

$$\tau_{\mathbf{1}}^{\pm}{}_{\mathbf{1}}A\tau_{\mathbf{1}}^{\mp}{}_{\mathbf{1}} = \tau_+A\tau_- + \tau_-A\tau_+ + \tau_{\mathbf{1}}A\tau_{\mathbf{1}} + \tau_{\mathbf{1}}A\tau_{\mathbf{1}},$$

an explicit representation of the projectors is

$$\tau_+ = \frac{i}{2}(\tau_{\mathbf{1}} + i\tau_2)\sigma_2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\tau_{\mathbf{1}} = \frac{i}{2}(1+\tau_3)\sigma_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

$$\tau_- = \frac{i}{2}(\tau_{\mathbf{1}} - i\tau_2)\sigma_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$\tau_{\mathbf{1}} = \frac{i}{2}(1-\tau_3)\sigma_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}.$$

Here, σ_α, $\alpha = 0,1,2,3$, is a quaternion subalgebra represented by the space-time multivectors $\{\mathbf{1},i\gamma_{23},i\gamma_{31},i\gamma_{12}\}$ such that in chiral representation they have the matrix representation

$$\sigma_\alpha = \left\{\begin{pmatrix}1&0\\0&1\end{pmatrix};\begin{pmatrix}\sigma_{\text{Pauli}} & 0\\ 0 & \sigma_{\text{Pauli}}\end{pmatrix}\right\}.$$

Then the τ_β, $\beta = 0,1,2,3$, are SU(2) gauge group generators represented here by the multivectors $\{\mathbf{1},\gamma_0,\gamma_{123},i\gamma_5\}$ such that in chiral representation they correspond to the supermatrices

$$\left\{\begin{pmatrix}1&0\\0&1\end{pmatrix},\begin{pmatrix}0&1\\1&0\end{pmatrix},\begin{pmatrix}0&-i\mathbf{1}\\ i\mathbf{1}&0\end{pmatrix},\begin{pmatrix}1&0\\0&-\mathbf{1}\end{pmatrix}\right\}.$$

(ii) The quaternion basis (σ^0,σ^j) is the Pauli matrix representation for the proper Lorentz group and (Σ^0,Σ^j) are the Proca matrix representation for the spin 1 proper Lorentz group given by

$$\Sigma^0 = \begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{pmatrix}, \quad \Sigma^1 = \begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&-i\\0&0&i&0\end{pmatrix},$$

$$\Sigma^2 = \begin{pmatrix}0&0&0&0\\0&0&0&i\\0&0&0&0\\0&-i&0&0\end{pmatrix}, \quad \Sigma^3 = \begin{pmatrix}0&0&0&0\\0&0&-i&0\\0&i&0&0\\0&0&0&0\end{pmatrix}.$$

(iii) In the left-hand side the term

$$((i/2)B^0_0(\psi,\psi)P_a + \tfrac{1}{4}B^0_\beta(\psi,\psi)\tau_j\tau^\beta\tau_j P_b)$$

is a factor produced by the use of the generalized Fierz identity[15] and the new time-space components those that were defined when the quaternion basis was changed, using

$$P_a = \mathbf{1} \text{ and } P_b = \begin{pmatrix}0&1\\0&0\end{pmatrix}.$$

An interpretation of this factor is as a rotation operator applied on a basis set, it generates a new basis set up to a phase factor given by a scalar and a multivector reflected in a j axis ($B^0_0(\psi,\psi) = \psi^T\epsilon\psi$ and $B^0_\beta(\psi,\psi) = \psi^T\tau^*_\beta\epsilon\psi$).[5]

In fact, we have used in (2.8) the SU(2) gauge group in a quaternion basis representation spin 1 of the proper Lorentz group (the components of this basis are rotated on the previous ones given by the Pauli spin 1/2 proper Lorentz group) for the differential operator and finally we projected the quaternion subalgebra of the $M_\alpha,(\psi,\psi)$ multivector Cartan map in the original equation.

To analyze Eq. (3.2) we need to study each of its terms. Its left-hand side term can be written as

$$\tau_{\uparrow}^{\pm}{}_{\downarrow}\left[iB_0^0(\psi,\psi)\tau_i\tau^0 M_0(D^0\psi,\psi)\sigma_0\sigma^0\right.$$
$$+\tfrac{1}{4}B_\beta^0(\psi,\psi)\tau_j\tau^\beta\tau_j\tau_i\tau^j M_{j'}(\bar{\psi},D^K\psi)\sigma_{K'}\sigma^{k'}\delta_{JK}^{j'k'};$$
$$\left.B_0^0(\psi,\psi)\tau_i\tau^j M_{j'}(\psi,D^K\psi)\sigma_{K'}\sigma^{K'}\delta_{JK}^{J'K'}\right]\tau_{\uparrow}^{\mp}{}_{\downarrow}\begin{pmatrix}\Sigma_0\\ \Sigma_j\end{pmatrix}, \tag{3.3}$$

where the P_a and P_b projectors mix the (σ^0,σ^i) basis components obtaining a new (Σ^0,Σ^i) basis set. The last expression can be changed to

$$B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_i M_0(D^0\psi,\psi)\Sigma_0$$
$$+\tau_{\uparrow}^{\pm}{}_{\downarrow}(B_0^0(\psi,\psi),(i/4)B_\beta^0(\psi,\psi)\tau_j\tau^\beta\tau_j)$$
$$\times\tau_i\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\begin{bmatrix}\Sigma_k\\ \Sigma_0\end{bmatrix}, \tag{3.4}$$

which is equivalent to

$$B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_i M_0(D^0\psi,\psi)\Sigma_0$$
$$+B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_i\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}$$
$$\times\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_K+\tau_{\uparrow}^{\pm}{}_{\downarrow}(\tfrac{1}{4}B_\beta^0(\psi,\psi)\tau_j\tau^\beta\tau_K\tau^j$$
$$\times M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'})\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0 \tag{3.5}$$

because τ_i,τ_j, and τ_K satisfy the SU(2) Lie algebra.

Due to (2.3) and $B_\beta^0(\psi,\psi)\tau_j\tau^\beta\tau_K=B_{J_\alpha}^0\tau^{\alpha T}\tau_K$, where $B_{J_\alpha}^0=(\psi^T\tau_3\tau_j^T\tau_\alpha\tau_3\epsilon\psi)$, expression (3.5) can be written as

$$B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}M_i(D^0\psi,\psi)\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0$$
$$+B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_i\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_K$$
$$+\tfrac{1}{4}\tau_{\uparrow}^{\pm}{}_{\downarrow}(B_{J_\alpha}^0\ \tau_\alpha^T)\tau_K\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0, \tag{3.6}$$

which is equivalent to

$$B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}M_i(D^0\psi,\psi)\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0+B_0^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_i\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_K$$
$$+\tfrac{1}{4}B_{j_0}^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_K\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0+\tfrac{1}{4}B_{j_1}^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_1\tau_k\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0$$
$$-\tfrac{1}{4}B_{j_2}^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_2\tau_k\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0+\tfrac{1}{4}B_{j_3}^0(\psi,\psi)\tau_{\uparrow}^{\pm}{}_{\downarrow}\tau_3\tau_k\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}\tau_{\uparrow}^{\mp}{}_{\downarrow}\Sigma_0. \tag{3.7}$$

Taking the transpose (3.7) and using (2.3), we obtain

$$\tfrac{1}{2}B_0^0(\psi,\psi)D^\alpha\Sigma_\alpha\tau_{\uparrow}^{\pm}{}_{\downarrow}M_i^T(\psi,\psi)\tau_{\uparrow}^{\mp}{}_{\downarrow}+\tfrac{1}{4}\Sigma_0(\tau_{\uparrow}^{\pm}{}_{\downarrow}B_{J_0}^0(\psi,\psi)M_K^T(D\psi,\psi)\tau_{\uparrow}^{\mp}{}_{\downarrow})$$
$$+\tfrac{1}{4}\Sigma_0(\tau_{\uparrow}^{\pm}{}_{\downarrow}B_{J_1}^0(\psi,\psi)M_K^T(D\psi,\psi)\tau_1\tau_{\uparrow}^{\mp}{}_{\downarrow})+\tfrac{1}{4}\Sigma_0(\tau_{\uparrow}^{\pm}{}_{\downarrow}B_{J_2}^0(\psi,\psi)M_K^T(D\psi,\psi)\tau_2\tau_{\uparrow}^{\mp}{}_{\downarrow})$$
$$+\tfrac{1}{4}\Sigma_0(\tau_{\uparrow}^{\pm}{}_{\downarrow}B_{J_3}^0(\psi,\psi)M_K^T(D\psi,\psi)\tau_3\tau_{\uparrow}^{\mp}{}_{\downarrow}). \tag{3.8}$$

About this expression the following comments are of interest:

(i) the $(\tau_{\uparrow}^{\pm}{}_{\downarrow}M\tau_{\uparrow}^{\mp}{}_{\downarrow})$ operator which obtains the quaternion part of a multivector M is equal to its transpose because

$\tau_+^T=-\tau_-,\tau_\uparrow^T=-\tau_\uparrow$, and $(\tau_\uparrow)^T=-\tau_\uparrow$.

(ii) The Proca matrices are such that

$\Sigma_0^T=\Sigma_0,\Sigma_i^T=-\Sigma_i$, with $i=1,2,3$.

(iii) Using (2.3), it is possible to prove

$\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}=M_0(D^K\psi,\psi)$, for $k=1,2,3$.

Then, if $\mathbf{D}=(D^1,D^2,D^3)$ the previous expression is equivalent to

$\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}=M_0(\mathbf{D}\psi,\psi)$

and

$\tau_i\tau^j M_{j'}(D^K\psi,\psi)\delta_{JK}^{J'K'}=\tau_i M_0(\mathbf{D}\psi,\psi)=M_i(\mathbf{D}\psi,\psi)$.

(iv) The τ_i $(i=1,2,3)$ matrices satisfy the Lie algebra $\tau_i\tau_j=i\tau_k$, with i,j,k cyclic.

The following properties[7] of the operators $(\tau_{\uparrow}^{\pm}{}_{\downarrow},\tau_{\uparrow}^{\mp}{}_{\downarrow})$:

$\tau_\pm\tau_3=\mp\tau_\pm$, $\tau_3\tau_\pm=\pm\tau_\pm$,

$\tau_{\uparrow\downarrow}\tau_3=\pm\tau_{\uparrow\downarrow}$, $\tau_3\tau_{\uparrow\downarrow}=\pm\tau_{\uparrow\downarrow}$,

$\tau_2\tau_\pm=\pm i\tau_{\downarrow\uparrow}$, $\tau_\pm\tau_2=\pm i\tau_{\downarrow\uparrow}$,

$\tau_2\tau_{\uparrow\downarrow}=\pm i\tau_\mp$, $\tau_{\uparrow\downarrow}\tau_2=\mp i\tau_\pm$,

$\tau_1\tau_\pm=\tau_{\downarrow\uparrow}$, $\tau_\pm\tau_1=\tau_{\downarrow\uparrow}$,

$\tau_1\tau_{\uparrow\downarrow}=\tau_\mp$, $\tau_{\uparrow\downarrow}\tau_1=\tau_\pm$,

can be used to transform expression (3.8) into

$$\tfrac{1}{2}B^0_0(\psi,\psi)D^\alpha\Sigma_\alpha(\tau_+ M^T_i(\psi,\psi)\tau_- + \tau_- M^T_i(\psi,\psi)\tau_+ + \tau_\uparrow M^T_i(\psi,\psi)\tau_\uparrow + \tau_\downarrow M^T_i(\psi,\psi)\tau_\downarrow)$$
$$+ \tfrac{1}{4}\Sigma_0(\tau_+ B^0_{j_0}M^T_k(\mathbf{D}\psi,\psi)\tau_- + \tau_- B^0_{j_0}M^T_k(\mathbf{D}\psi,\psi)\tau_+ + \tau_\uparrow B^0_{j_0}M^T_k(\mathbf{D}\psi,\psi)\tau_\uparrow + \tau_\downarrow B^0_{j_0}M^T_k(\mathbf{D}\psi,\psi)\tau_\downarrow)$$
$$+ \tfrac{1}{4}\Sigma_0(\tau_- B^0_{j_\downarrow}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_\downarrow + \tau_+ B^0_{j_\uparrow}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_\uparrow + \tau_\uparrow B^0_{j_\uparrow}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_-$$
$$+ \tau_\downarrow B^0_{j_\downarrow}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_+) + (i/4)\Sigma_0(\tau_\uparrow B^0_{j_2}M^T_k(\mathbf{D}\psi,\psi)\tau_- - \tau_\downarrow B^0_{j_2}M^T_k(\mathbf{D}\psi,\psi)\tau_+ + \tau_- B^0_{j_2}M^T_k(\mathbf{D}\psi,\psi)\tau_\downarrow$$
$$- \tau_+ B^0_{j_2}M^T_k(\mathbf{D}\psi,\psi)\tau_\uparrow) + \tfrac{1}{4}\Sigma_0(\tau_\uparrow B^0_{j_3}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_\uparrow - \tau_\downarrow B^0_{j_3}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_\downarrow$$
$$+ \tau_- B^0_{j_3}M^T_k(\mathbf{D}\psi,\psi)\tau_+ - \tau_+ B^0_{j_3}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi)\tau_-). \tag{3.9}$$

Due to (2.3) the multivectorial Cartan map is lineal and symmetric[4]

$$OM_\beta(\psi,\psi) = M_\beta(\hat{O}\psi,\psi) = M_\beta(\psi,\hat{O}\psi),$$

where O is an operator (differential or not) over the multivector space while $\hat{O}$ is its equivalent on the spinor space. Thus,

$$M^T_j(D\psi,\psi)M^T_k(\psi,\psi) = 16\tau_3\epsilon(\mathbf{D}\psi)\psi^T\tau_3\tau^T_j\tau_3\epsilon\psi\psi^T\tau_3\tau^T_k,$$

equivalently,

$$M^T_j(\psi,D\psi)M^T_k(\psi,\psi) = 16\tau_3\epsilon\psi\mathbf{D}\psi^T\tau_3\tau^T_j\tau_3\epsilon\psi\psi^T\tau_3\tau^T_k.$$

Here, we will use the first expression that is equivalent to

$$M^T_j(\mathbf{D}\psi,\psi)M^T_k(\psi,\psi) = 4(\psi^T\tau_3\tau^T_j\tau_3\epsilon\psi)(4\tau_3\epsilon(\mathbf{D}\psi)\psi^T\tau_3\tau^T_k) = 4B^0_{j_0}(\psi,\psi)M^T_k(\mathbf{D}\psi,\psi).$$

It is possible in general to show that

$$M^T_j(\mathbf{D}\psi,\psi)\tau_\alpha M^T_k(\psi,\psi) = (\psi^T\tau_3\tau^T_j\tau_\alpha\tau_3\epsilon\psi)M^T_k(\mathbf{D}\psi,\psi) = B^0_{j_\alpha}M^T_k(\mathbf{D}\psi,\psi). \tag{3.10}$$

Using (3.10) and (3.9) we obtain for (3.3)

$$\tfrac{1}{2}B^0_0(\psi,\psi)D^\alpha\Sigma_\alpha(\tau_+ M^T_i(\psi,\psi)\tau_- + \tau_- M^T_i(\psi,\psi)\tau_+ + \tau_\uparrow M^T_i(\psi,\psi)\tau_\uparrow + \tau_\downarrow M^T_i(\psi,\psi)\tau_\downarrow)$$
$$+ \tfrac{1}{4}\Sigma_0(\tau_+ M^T_j(\mathbf{D}\psi,\psi)M^T_k(\psi,\psi)\tau_- + \tau_- M^T_j(\mathbf{D}\psi,\psi)M^T_k(\psi,\psi)\tau_+ + \tau_\uparrow M^T_j(\mathbf{D}\psi,\psi)M^T_k(\psi,\psi)\tau_\uparrow$$
$$+ \tau_\downarrow M^T_j(\mathbf{D}\psi,\psi)M^T_k(\psi,\psi)\tau_\downarrow) + \tfrac{1}{4}\Sigma_0(\tau_+ M^T_j(D\psi,\psi)\tau_\uparrow M^T_k(\psi,\psi)\tau_\uparrow + \tau_- M^T_j(\mathbf{D}\psi,\psi)\tau_\uparrow M^T_k(\psi,\psi)\tau_\downarrow$$
$$+ \tau_\uparrow M^T_j(\mathbf{D}\psi,\psi)\tau_\uparrow M^T_k(\psi,\psi)\tau_- + \tau_\downarrow M^T_j(\mathbf{D}\psi,\psi)\tau_\uparrow M^T_k(\psi,\psi)\tau_+) + (i/4)\Sigma_0(\tau_\uparrow M^T_j(\mathbf{D}\psi,\psi)\tau_2 M^T_k(\psi,\psi)\tau_-$$
$$- \tau_\downarrow M^T_j(\mathbf{D}\psi,\psi)\tau_2 M^T_k(\psi,\psi)\tau_+ + \tau_- M^T_j(\mathbf{D}\psi,\psi)\tau_2 M^T_k(\psi,\psi)\tau_\downarrow - \tau_+ M^T_j(\mathbf{D}\psi,\psi)\tau_2 M^T_k(\psi,\psi)\tau_\downarrow)$$
$$+ \tfrac{1}{4}\Sigma_0(\tau_\uparrow M^T_j(\mathbf{D}\psi,\psi)\tau_3 M^T_k(\psi,\psi)\tau_\uparrow - \tau_\downarrow M^T_j(\mathbf{D}\psi,\psi)\tau_3 M^T_k(\psi,\psi)\tau_\downarrow$$
$$+ \tau_- M^T_j(\mathbf{D}\psi,\psi)\tau_3 M^T_k(\psi,\psi)\tau_+ - \tau_+ M^T_j(\mathbf{D}\psi,\psi)\tau_3 M^T_k(\psi,\psi)\tau_-), \tag{3.11}$$

which is equivalent to writing (3.3) in the form

$$\tfrac{1}{2}B^0_0(\psi,\psi)D^\alpha\Sigma_\alpha(\tau_+ M^T_i(\psi,\psi)\tau_- + \tau_- M^T_i(\psi,\psi)\tau_+ + \tau_\uparrow M^T_i(\psi,\psi)\tau_\uparrow + \tau_\downarrow M^T_i(\psi,\psi)\tau_\downarrow)$$
$$+ \tfrac{1}{4}\Sigma_0[\tau_\uparrow M^T_j(D\psi,\psi)(1+\tau_3)M^T_k\tau_\uparrow + \tau_\uparrow M^T_j(D\psi,\psi)(\tau_\uparrow + i\tau_2)M^T_k(\psi,\psi)\tau_-$$
$$+ \tau_\downarrow M^T_j(D\psi,\psi)(1-\tau_3)M^T_k(\psi,\psi)\tau_\downarrow + \tau_\downarrow M^T_j(D\psi,\psi)(\tau_\uparrow - i\tau_2)M^T_k(\psi,\psi)\tau_+$$
$$+ \tau_- M^T_j(D\psi,\psi)(\tau_\uparrow + i\tau_2)M^T_k(\psi,\psi)\tau_\downarrow + \tau_- M^T_j(D\psi,\psi)(1+\tau_3)M^T_k(\psi,\psi)\tau_+$$
$$+ \tau_+ M^T_j(D\psi,\psi)(\tau_\uparrow - i\tau_2)M^T_k(\psi,\psi)\tau_\uparrow + \tau_+ M^T_j(D\psi,\psi)(1-\tau_3)M^T_k(\psi,\psi)\tau_-]. \tag{3.12}$$

Using the properties of the operator $(\tau^\pm_\uparrow,\tau^\mp_\uparrow)$, the expression (3.12) can be written as

$$\tfrac{1}{2}B^0_0(\psi,\psi)D^\alpha\Sigma_\alpha\tau^\pm_\uparrow M^T_i(\psi,\psi)\tau^\mp_\uparrow$$
$$- \tfrac{1}{2}\Sigma_0(\tau^\pm_\uparrow M^T_j(\mathbf{D}\psi,\psi)\tau^\mp_\uparrow)(\tau^\pm_\uparrow M^T_k(\psi,\psi)\tau^\mp_\uparrow) \tag{3.13}$$

in a shorter notation. Given that the multivectorial map is linear and symmetric we can now write (3.13) as

$$\tfrac{1}{2}B^0_0(\psi,\psi)D^\alpha\Sigma_\alpha\tau^\pm_\uparrow M^T_i(\psi,\psi)\tau^\mp_\uparrow$$
$$- \tfrac{1}{4}[\mathbf{D}\Sigma_0(\tau^\pm_\uparrow M^T_j(\psi,\psi)\tau^\mp_\uparrow)(\tau^\pm_\uparrow M^T_k(\psi,\psi)\tau^\mp_\uparrow)]. \tag{3.14}$$

Here the indexes i,j,k must be cyclic.

To continue the transformation of (3.3) we now use an expression for the $B_\alpha(\psi,\psi')$. In a recent[7] paper we proved that the $B_\alpha(\psi,\psi') = B^\beta_\alpha(\psi,\psi')\sigma_\beta$ quaternion map can be obtained as

$$B_\alpha(\psi,\psi') = -\tfrac{1}{2}(\tau_\uparrow M^T_\alpha(\psi,\psi')\tau_\uparrow + \tau_\downarrow M^T_\alpha(\psi,\psi')\tau_\downarrow$$
$$+ \tau_+ M^T_\alpha(\psi,\psi')\tau_- + \tau_- M^T_\alpha(\psi,\psi')\tau_+),$$

where $B^\beta_\alpha(\psi,\psi') = \psi^T\sigma^\alpha\tau^*_\beta\epsilon\psi'$; thus, this method projects the quaternion subalgebra of $M_\alpha(\psi,\psi')\in\mathscr{C}(1,3)$ as basis space (space-time symmetry) for the SU(2) gauge group as isotopic space [τ_β are the SU(2) generators]. Consequently, we can identify

$$B_\alpha(\psi,\psi) = -\tfrac{1}{2}(\tau_\uparrow^{\pm}{}_\downarrow M_\alpha^T(\psi,\psi)\tau_\uparrow^{\mp}{}_\downarrow),$$

then (3.14) changes to

$$-B_0^0(\psi,\psi)D^\alpha\Sigma_\alpha B_i(\psi,\psi) - (\mathbf{D}\Sigma_0 B_j(\psi,\psi))\cdot B_k(\psi,\psi).$$

On the other hand, $D^\alpha\Sigma_\alpha B_i(\psi,\psi)$ is equivalent to $-iD^\alpha S_\alpha F_i$, where S^α is an irreducible representation (in fact, it is the spin-1 Proca representation) for the proper Lorentz group

$$S^0=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad S^1=\begin{pmatrix}0&0&0\\0&0&-i\\0&i&0\end{pmatrix},$$

$$S^2=\begin{pmatrix}0&0&i\\0&0&0\\-i&0&0\end{pmatrix},\quad S^3=\begin{pmatrix}0&-i&0\\i&0&0\\0&0&0\end{pmatrix}.$$

Moreover, for the quaternion $B_\alpha(\psi,\psi)$ the no null subspace is given by $F_j = i[B_j^1(\psi,\psi),B_j^2(\psi,\psi),B_j^3(\psi,\psi)]$. In the same way the $(\mathbf{D}\Sigma_0 B_j(\psi,\psi))\cdot B_k(\psi,\psi)$ term is equivalent to $-(\mathbf{D}F_j)\cdot F_k$. Consequently we can write the expression (3.14) of (3.3) as

$$-B_0^0(\psi,\psi)D^\alpha S_\alpha F_i + (DF_j)\cdot F_k, \tag{3.15}$$

which contains the F_i multivector fields on a $\mathcal{C}(1,3)$ space-time symmetry as basis space (if we would have used the quaternion space-time basis these fields would have been vector fields).

The transpose of the (3.2) left-hand side term is (3.15), its right-hand side term is

$$-\tau_\uparrow^{\pm}{}_\downarrow[(iB_0^0(\psi,\psi)/2)\phi^\beta\tau_\beta M_i(\psi,\bar\psi)]\tau_\uparrow^{\mp}{}_\downarrow$$

which is equivalent to

$$(-iB_0^0(\psi,\psi)/2)\tau_\uparrow^{\pm}{}_\downarrow[\phi^\beta\tau_\beta M_i(\psi,\bar\psi)]\tau_\uparrow^{\mp}{}_\downarrow \tag{3.16}$$

or

$$(i/2)B_0^0(\psi,\psi)\tau_\uparrow^{\pm}{}_\downarrow[\phi_i M_0(\psi,\bar\psi) + i\epsilon_{imn}\phi_m M_n(\psi,\bar\psi)]\tau_\uparrow^{\mp}{}_\downarrow, \tag{3.17}$$

as far as the component ϕ^0 is always null, and ϵ_{imn} is the antisymmetric tensor.

The transpose of (3.17) is

$$(i/2)B_0^0(\psi,\psi)\tau_\uparrow^{\pm}{}_\downarrow[\phi_i M_0^T(\psi,\bar\psi) + i\epsilon_{kmn}\phi_m M_n^T(\psi,\bar\psi)]\tau_\uparrow^{\mp}{}_\downarrow$$

or

$$(i/2)B_0^0(\psi,\psi)\phi_i\tau_\uparrow^{\pm}{}_\downarrow M_0^T(\psi,\bar\psi)\tau_\uparrow^{\mp}{}_\downarrow + i\epsilon_{kmn}\phi_m\tau_\uparrow^{\pm}{}_\downarrow M_n^T(\psi,\bar\psi)\tau_\uparrow^{\mp}{}_\downarrow \tag{3.18}$$

using $B_\alpha(\psi,\bar\psi) = -\tfrac{1}{2}\tau_\uparrow^{\pm}{}_\downarrow M_\alpha^T(\psi,\bar\psi)\tau_\uparrow^{\mp}{}_\downarrow$, we obtain

$$J_i = -iB_0^0(\psi,\psi)[B_0(\psi,\bar\psi)\phi_i + i\epsilon_{kmn}\phi_m B_n(\psi,\bar\psi)]. \tag{3.19}$$

From all the transformations above, Eq. (3.2) can be finally written as

$$D^\alpha S_\alpha F_i + i((DF_j)\cdot F_k/B_0^0(\psi,\psi)) = B_0(\psi,\bar\psi)\phi_i + i\epsilon_{kmn}\phi_m B_n(\psi,\bar\psi), \tag{3.20}$$

which is the equation that was studied by F. Reifler,[4-6] applying it to electroweak interactions; we must remark that in our structure, the $B_\alpha(\psi,\chi)$ map is the $M_\alpha(\psi,\chi)$ projection in a quaternion space-time basis subalgebra of $\mathcal{C}(1,3)$ as sis space for the SU(2) gauge group used in an isotopic space. Here, (3.20) have been obtained changing the representation of the differential operator (in order to go from spin 1/2 to spin 1 functions of the proper Lorentz group), the new components are a rearrangement of the old ones. This definition of a new basis in the differential operator produces the projection of $B_i(\psi,\psi)$ into $F_i(\psi,\psi)$ in a subalgebra of the quaternion algebra [which is a subalgebra of $\mathcal{C}(1,3)$] only for the left-hand side term of (3.20)) (right-hand side does not have differential operators and, consequently, it is written in all the quaternion algebra).

IV. DISCUSSION

(i) The extended Cartan map given in (2.3)

$$M_\beta^\alpha(\psi,\psi') = \psi^T\Gamma^\alpha(\overline{\lambda_\beta\psi'^*}) = \psi^T\Gamma^\alpha\bar\lambda_\beta\epsilon\psi'$$

does not change when we transform the minimum ideals of $\mathcal{C}(1,3)$, ψ and χ (spinors, elements of C^4) using infinitesimal gauge rotations only if $\epsilon\omega_i = -\omega_i^T\epsilon$ and $\Gamma^\alpha\bar\lambda_\beta\theta_i\omega^{iT} = \theta_i\omega^{iT}\Gamma^\alpha\bar\lambda_\beta$ (ω_i is a gauge group generator and θ_i is its associated phase). In particular the $B_\beta^\alpha(\psi,\psi')$ quaternion map projected from the $M_\beta^\alpha(\psi,\psi')$ map satisfies the previous conditions when the SU(2) gauge group is used.

The (2.3) map over the minimum ideals ψ,χ is invariant under the Lorentz transformations if $\gamma_{\alpha\beta}^T\Gamma^\alpha\bar\lambda_\beta\epsilon = -\Gamma^\alpha\bar\lambda_\beta\epsilon\gamma_{\alpha\beta}$ with $\alpha,\beta = 0,1,2,3$ ($\gamma_{\alpha\beta}$ is the multivector representation of the generators of the proper Lorentz group); besides, the CPT operator applied on the χ,ψ minimum ideals transforms the extended Cartan map as

$$M_\beta^\alpha(\mathrm{CPT}\,\psi(x,t),\mathrm{CPT}\,\chi(x,t)) = e^{-i\pi}M_\beta^\alpha[\psi(-x,-t),\chi(-x,-t)]. \tag{4.1}$$

Finally, we must remark that the multivector map $M_\beta(\psi,\chi)$ [or the extended Cartan map $M_\beta^\alpha(\psi,\chi)$] is defined over two Hilbert spaces given by the χ and ψ minimum ideals that in this case correspond to Dirac solutions of a Dirac equation.

(ii) The projection method used here to obtain the $B_\alpha(\psi,\psi')$ quaternion map from the $M_\alpha(\psi,\psi,')$ map shows that the quaternion projection of $B_\alpha(\psi,\psi')$ is in itself. The physical content of a Lagrangian that is a function of quaternion fields does not change with (quaternion) operations that preserve the algebra. This automorphism was studied by Birkhoff, von Newman,[16] and Finkelstein[17,18] in their quaternionic quantum mechanics (QQM). Our structure is different than these works because their gauge transformation is presented as a particular case of a quaternion subalgebra projection [in general we projected $\mathcal{C}(1,3)$ to quaternions but it is always possible a quaternion–quaternion projection]. Moreover, we can include different physical situations in the same logical structure. On the other hand, in QQM the physical fields are considered as the components of the quaternionic fields. Here, we consider them as a $M_\alpha(\psi,\psi)$ multivector. (A gauge transformation in QQM rotate the physical fields of particles among themselves while in the second interpretation the multivector fields are transformed into themselves.)[19] As yet, the QQM cannot clearly originate a supersymmetric theory of fermionic and

bosonic fields.

(iii) In a recent paper[15] we showed that the Clifford product for $B_j(\psi,\chi)$ quaternion maps satisfies the following structure:

$$B_J(\psi,\chi)B_k(\chi',\psi') = C^{PQ}_{JK}B^0_P(\psi,\psi')B_Q(\chi',\chi),$$

with $C^{JKPQ} = g^{JP}g^{KQ} + g^{JQ}g^{KP} - g^{JK}g^{PQ} - i\epsilon^{JKPQ}$, where g^{JK} is the Lorentz's metric tensor; ϵ^{JKPQ} is the full antisymmetric permutation tensor; $\psi,\psi',\chi,\chi' \in C^4$ are left minimum ideals of $\mathscr{C}(1,3)$.

If $\psi = \psi' = \chi = \chi'$ and we use only the no null subspace, we obtain

$$iB^0_0(\psi,\psi) = (F_i x F_j \cdot F_k)/\lambda, \text{ where } \lambda = \|F_i\|;\ i,j,k \text{ cyclic.} \tag{4.2}$$

This expression has nine degrees of freedom and gives the ψ structure, using its bilineal forms [The $M_\alpha(\psi,\psi)$ map from $C^4 \times C^4$ to $\mathscr{C}(1,3)$ is fourfold covering over $B_\alpha(\psi,\psi)$ for each isotopic direction with ten non-null extended Cartan maps.[7]] On the other hand, if we use a chiral representation for the $\mathscr{C}(1,3)$ multivectors and assign a particular value to its minimum ideal ψ (spinor)[2,9] such that represents a particle without Dirac mass, the F_i ($i = 1,2$ because $F_3 \equiv 0$) fields are the same as those that represent the electromagnetic field written in a quaternion algebra:

$$-\frac{1}{i}\sum_{j=0}^{3}\alpha^j\frac{\partial}{\partial x^j}\psi = 4\pi\Phi$$

with

$$\psi = \begin{pmatrix} 0 \\ H_x - iE_x \\ H_y - iE_y \\ H_z - iE_z \end{pmatrix},\quad \Phi = \begin{pmatrix} 0 \\ J_x \\ J_y \\ J_z \end{pmatrix}, \text{ and}$$

$$\alpha^j = \left\{ 1, \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & i \\ -1 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} \right\}, \tag{4.3}$$

studied by Moses[20] (see references therein). When we have two polarized electromagnetic waves in the Z direction (for F_1; $E_y = H_x = 0$ and $E_x = H_y$ while for F_2; $H_x = -E_y$ and $E_x = H_y = 0$), this construction reminds us of that having its origin in the photon neutrino duality, the old idea to construct photons from neutral massless Dirac fields (usually called neutrino pairs).[21]

(iv) The structure presented in this paper can be used to construct the Lagrangians. In general it is possible to find out all the combinations that do not change when we apply the multivectorial Cartan map and use them to construct a Lagrangian with the Noether currents and dynamical equations wanted. This Lagrangian could include multivector fields that are given by the gauge group algebra on the $\mathscr{C}(1,3)$ space-time group.

As a matter of fact, we can construct a Lagrangian using $M_\alpha(\psi,\chi)$ multivector map [for example with SU(2) gauge group as isotopic symmetry]; then, if wanted, we could project it into its quaternion subalgebra giving the $B_\alpha(\psi,\chi)$ quaternion map. This allows the QQM with an additional concept: the spontaneous symmetry breaking on the spacetime symmetry, similar to the well known Higgs mechanism on the isotopic space for the QQM.[19]

(v) When we proposed Eq. (2.2) we used the $\phi^\alpha = (0,0,0,m)$ value to reproduce the electron Dirac equation, now if we assign a different value (following Reifler's analysis[4-6]) $\phi^\alpha = (0,m',0,0)$; then (2.2) changes to

$$P^\alpha\tau_\alpha\xi = m'\bar{\xi},\quad P^\alpha\tau_\alpha\eta = -m'\bar{\eta}, \tag{4.4}$$

where $\psi = \begin{pmatrix}\xi \\ \eta\end{pmatrix}$ is the spinor associated to the new ϕ^α. For $m' \to 0$, the (4.4) system corresponds to a particle that will be called neutrino.

Consequently a chosen set ϕ^β gives elements to associate it with an elementary particle, as follows we will use $\hat{\phi}^\beta = \phi^\beta/m = (0,0,0,1)$ for the neutrino (it is not possible in this initial scheme to reflect the differences between families). As the $\hat{\phi}^\beta$ satisfy the SU(2) algebra when we assign a $\hat{\phi}^\beta$ value to an elementary particle we are giving it a particular isotopic direction in the SU(2) gauge space; this is a way to assign mass alternative to the usual Higgs mechanism (then it is always necessary that $\phi^0 = 0$).

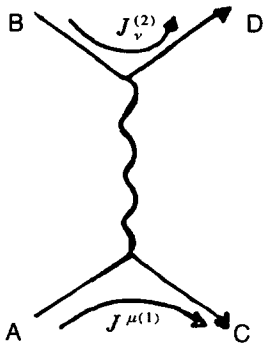
(iv) To study particle interactions we may, as usual, write the differential cross section, in the symbolic form[9]

$$d\sigma = (|M^2|/F)dQ, \tag{4.5}$$

where M is the invariant amplitude that contains the significant physical information and is giving by the Feynman rules associated to the interaction diagram, dQ is the Lorentz invariant phase space factor, and F is the incident flux in the laboratory. In the following analysis we will only use M because the physics resides in it.

In perturbation theory, in its lowest-order Feynman diagram with scalar propagators, the Feynman rules for the invariant amplitude M associated with a particular interaction between elementary particles gives the following expression:

$$iM = \left(ie\bar{u}_c\gamma^\mu\frac{1}{2}(1-\gamma^5\omega)u_A\right)\frac{g^v_\mu}{p^2 - m^2_\omega} \times\left(ie\bar{u}_D\gamma_v\frac{1}{2}(1-\gamma_5\omega)u_B\right), \tag{4.6}$$



for the interaction diagram
$J^{\mu(1)} = ie\bar{u}_c\gamma^\mu \tfrac{1}{2}(1-\gamma^5\omega)u_A$,
$J_\nu^{(2)} = ie\bar{u}_D\gamma_\nu \tfrac{1}{2}(1-\gamma_5\omega)u_B$,
g_μ^ν is the Lorentz tensor metric,

with u_i as the Dirac bispinor associated to the i fermion. The ω factor is null if the interaction is vectorial (QED) and one when there are vector and axial currents in the theory (electroweak interaction). Finally $g_\mu^\nu/(p^2-m_\omega^2)$ is the scalar propagator with p the moment and m_ω the mass that is null if $\omega=0$. This particular case relates the multivector Cartan map with interaction diagrams in QED and electroweak process.

Using the multivector Cartan map, we propose the following expression for M under the previous conditions:

$$iM = \frac{e^2}{2}(1+i\gamma_5 \operatorname{sen}\theta_{Ac})(\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_A,\bar{\psi}_c)\tau_\uparrow^{\mp}{}_\downarrow)^\nu \times \frac{g_\nu^\mu}{p^2-m^2}(1+i\gamma_5 \operatorname{sen}\Theta_{BD}) \times(\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_B,\bar{\psi}_D)\tau_\uparrow^{\mp}{}_\downarrow). \tag{4.7}$$

In this expression the transition current associated to the A and B particles is obtained as the quaternion projection of the multivector map $M_0(\psi'_A,\bar{\psi}_B)$ written in two Hilbert spaces (given by the left minimum ideals associated to the A and B elementary particles) for different space-time positions. (We must remark that the multivector map does not have isotopic direction because in any of them the transition current cannot be developed in a quaternion subalgebra.) Finally θ_{AB} is the angle produced by the $\hat{\phi}_k(A)$ and $\hat{\phi}_k(B)$ isotopic directions. We will assume as follows that $\hat{\phi}_k$ will be additive and will conserve during an interaction. Thus, ϕ_k can be interpreted as a tag that let us express the usual conservative quantum numbers; baryon numbers, lepton number, and electric charge, in several ways for each particle (there is not an only way to assign them for a particle). We can construct a method to give mass for the gauge bosons. As the $\hat{\phi}_k$ numbers are additive which are conserved for each Feynman vertex, it is possible to get a $\hat{\phi}_k$ value associated with gauge bosons. The gauge bosons mass could be defined as a function of its $\|\hat{\phi}_k\|$. (Using this method, the model predicts the photon and gluon null mass and for W^+, W^-;Z the no null mass.)

For QED $\operatorname{sen}\theta_{AC} = \operatorname{sen}\theta_{BD} = 0$ and $m_\gamma = 0$; then (4.27) with $\omega=0$ is equivalent to (4.26). If we use $\operatorname{sen}\theta_{AC} = \operatorname{sen}\theta_{BD} = 1$ and $m_\omega \neq 0$ in (4.27). ($\omega=1$), we get the common invariant amplitude M for the electroweak process. In a general electroweak process (for example $e^- + W^+ \to \nu$, $u \to W^+ + d$ and $c \to W^+ + s$) the $\hat{\phi}_k(W^+)$ associated is given by $\hat{\phi}_k(W^+) = (0,1,0,-1)$. Thus, it is possible to obtain additional conditions over the $\hat{\phi}_k$ associated to elementary particles as a normalization restriction but we prefer to derive them from experimental facts, opposite to the Reifler and Morris work,[4-6] because only the $\hat{\phi}_k$ quaternions for elementary particles produced for physical experiments can give us significant information. Then the (4.27) invariant amplitude extended for C^8 minimum ideals in a SU(3) gauge symmetry is the only one which can explain the QCD model clearly.

Finally, to find out that a particular process like $K^+ \to \mu^+ + \nu_\mu$ and $\pi^+ \to \mu^+ + \nu_\mu$ does not explain with only one particular family, we proposed a state rotation between d and s quarks in a θ_c Cabibbo angle. The relation of invariant amplitude for the β strange decay ($s \to u + e + \bar{\nu}$) and the β decay ($d \to u + e + \bar{\nu}$) is defined as the $\tan\theta_c$, assuming (4.27) as true:

$$\tan\theta_c = \frac{(1+i\gamma_5 \operatorname{sen}\theta_{su})(\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_s,\bar{\psi}_u)\tau_\uparrow^{\mp}{}_\downarrow)^\nu[g_\nu^\mu/(p^2-m'^2)](\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_\nu,\bar{\psi}_e)\tau_\uparrow^{\mp}{}_\downarrow)_\mu}{(1+i\gamma_5 \operatorname{sen}\theta_{du})(\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_d,\bar{\psi}_u)\tau_\uparrow^{\mp}{}_\downarrow)^\nu[g_\nu^\mu/(p^2-m^2)](\tau_\uparrow^{\pm}{}_\downarrow M_0(\psi'_\nu,\bar{\psi}_e)\tau_\uparrow^{\mp}{}_\downarrow)_\mu}, \tag{4.8}$$

where $\operatorname{sen}\theta_{du} = 1$, thinking that $p^2 << m^2$ and $p^2 << m'^2$ (4.28) predicts $\operatorname{sen}\theta_{su} = 1$ and $m = \sqrt{\tan\theta_c}\,m' = 0.4837m'$.

In the previous paragraph we followed a particular interpretation. On the contrary, it is possible to assume other ways, for example, we could have defined the $\hat{\phi}_k$ quaternions associated to elementary particles elements (leptons and quarks) using particular invariant amplitudes [perhaps they would be different to (4.27)] and an m'/m relation fixed. Thus, we could have obtained a Cabibbo angle that was compared with the experimental value. However, this procedure cannot explain clearly the large quantity of suppositions included and it is contrary to our ideas. In the Reifler and Morris[6] vector model for electroweak interactions the $\bar{\phi}_k$ quaternions (called Higgs in their papers) are given according to the conserved numbers (electric charge, baryon number, and lepton number) definitions. Moreover, a Lagrangian (which has the common Noether currents and the usual movement Dirac equation) and an arbitrary transition matrix (in our structure the invariant amplitude is given in function of the multivector Cartan map in a very simple construction) allowing to obtain additional condition for these

$\hat{\phi}_k$ quaternions. Obviously our structure is more general than this one. [It is always possible to project the quaternion subalgebra of $\mathscr{C}(1,3)$ for an extended Cartan map with SU(2) gauge group and reduce the arbitrary suppositions involved in the model.]

(vi) The differential operator written in (2.2) [which produced the (2.8) multivector equation and its (3.20) projection] can be given by

$$\mathbf{D}^{\alpha} = ih\nabla^{\alpha} + eV_k^{\alpha} t^k + e_0 V_0^{\alpha} t^0, \tag{4.9}$$

where V_{β}^{α} $\beta = 0,k$ are directly observable Yang–Mills potentials. Equation (4.9) is a covariant derivative if t_{β} are Lie group generators.

Taking the SU(2) particular case of (4.29) e and e_0 are the absolute values of electric and neutral charges and this expression must be equivalent to the usual Weinberg–Salam covariant derivative

$$\mathbf{D}'^{\alpha} = ih\nabla^{\alpha} - gW_k^{\alpha} t'^k - g_0 W_0^{\alpha} t'^0, \tag{4.10}$$

where g and g_0 are the coupling coefficients, W_{β}^{α} are the Yang–Mills potentials in the Weinberg–Salam model (no directly observable).

The SU(2) generators t^{β} and t'^{β} are in different representations and the Weinberg–Salam angle will give their relation. Thus if $t_3 = -t'_3 - t'_0$ and $t_0 = -3t'_3 + t'_0$,

$$eV_3^{\alpha}(t'_3 + t'_0) + e_0 V_0^{\alpha}(3t_3 - t'_0) = gW_3^{\alpha} t^{3'} + g_0 W_0^{\alpha} t'_0,$$

due to

$$W_3^{\alpha} = V_0^{\alpha} \cos\theta_w + V_3^{\alpha} \operatorname{sen}\theta_w,$$

$$W_0^{\alpha} = -V_0^{\alpha} \operatorname{sen}\theta_w + V_3^{\alpha} \cos\theta_w.$$

Then

$$\tan\theta_w = \tfrac{1}{3}\cot\theta_w = g_0/g,$$

$$\operatorname{sen}^2\theta_w = \tfrac{1}{4}, \text{ and } e_0 = e\tan\theta_w,$$

which are close to the experimental values.[8,9]

(vii) The final comment is about the objections one could make against using multivectorial fields to describe fermionic and bosonic particles since the properties of the system are not apparent, but there are several ways to solve this problem.

Witten[22] has shown that there is a way around this problem. The idea was to add an abnormal term I to the SU(3) nonlinear σ- model Lagrangian $L = \text{const} \times \int d^{\nu} U \partial_{\nu} U * d^4 x$ such that $\exp iI(U)$ produces a factor -1 in the quantum mechanical action when $U(x,t)$ represents a soliton that is rotated by an angle 2π when the time t goes from $-\infty$ to ∞. Thus, it is possible to expect that a Lagrangian with multivectorial fields can be quantized in a desired form adding abnormal terms as in the Witten procedure.

On the other hand, Bacry and Boon[23] proposed a boson algebra and a symplectic Clifford algebra structure on $2n$ vector spaces where the canonical basis made of isotropic vectors, say $\{a, a_2,...,a_n, a_1^+, a_2^+,..., a_n^+\}$ (n creation operators and n destruction operators) is its generator basis. This form is useful if we can introduce the statistics of physical fields and its canonical quantization because for a simple case,[8]

$$\phi(x,t) = \int \frac{d^3k}{[(2\pi)^3 2\omega_k]^{1/2}} \times [a(k)e^{i(ik\cdot x - \omega_k t)} + a^+(k)e^{-i(k\cdot x - \omega_k t)}], \tag{4.11}$$

where the statistics for the physical field $\Phi(x,t)$ is given by the commutation relations of the $a(k)$ and $a^+(k)$ operators. When $\Phi(x,t)$ is a multivector field the operator $a(k)$ and $a^+(k)$ are also multivectors of the same Clifford algebra (symmetric or symplectic) which can be chosen.

V. CONCLUSIONS

We have shown the general procedure to obtain dynamical equations where the field representing the particle is a multivector, using the multivectorial generalization of the Cartan map in $\mathscr{C}(1,3)$ space-time Clifford group and any Lie gauge group in an isotopic space. The algebraic properties of this map and the generalized Fierz identities were applied to obtain a multivectorial Dirac equation. This multivectorial field can be defined on any manifold (with or without spin structure). In the Dirac case, it represents a fermionic field.

We obtained, as a particular case, the quaternion projection of the multivectorial Dirac equation with SU(2) Lie gauge group in the isotopic space which was related to a well-known equation for electroweak interactions.[5] The multivectorial structure of this equation and some properties and limitations (for example, the origin of the Proca representation for the differential operator basis) were shown.

Finally, we presented among others, the following remarkable relations in some models of quantum field theory.

(1) The transformation properties of the multivectorial Cartan map for gauge groups, Lorentz group, and CPT operator applied over minimum ideals (interpreted as spinor spaces).

(2) The relation of the quaternion projection method with gauge transformation in quaternionic quantum mechanics.[16–19]

(3) The photon-neutrino duality.

(4) Some experimental facts in elementary particles interactions using multivectorial Cartan map properties (Cabibbo and Weinberg–Salam angles, gauge boson masses for the first and second quarks families, etc.).

(5) The boson and fermion Clifford algebras.

Thus, our structure is more general than the earlier one reducing its arbitrary assumptions.

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A novel approach to the synthesis of nondispersive wave packet solutions to the Klein–Gordon and Dirac equations

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A systematic approach to the derivation of exact nondispersive packet solutions to equations modeling relativistic massive particles is introduced. It is based on a novel bidirectional representation used to synthesize localized Brittingham-like solutions to the wave and Maxwell's equations. The theory is applied first to the Klein–Gordon equation; the resulting nondispersive solutions can be used as de Broglie wave packets representing localized massive scalar particles. The resemblance of such solutions to previously reported nondispersive wave packets is discussed and certain subtle aspects of the latter, especially those arising in connection to the correct choice of dispersion relationships and the definition of group velocity, are clarified. The results obtained for the Klein–Gordon equation are also used to provide nondispersive solutions to the Dirac equation which models spin 1/2 massive fermions.

I. INTRODUCTION

A large body of work has been inspired recently by Brittingham's focus wave mode (FWM) solutions[1] to Maxwell's equations. Such solutions are built up of a Gaussian envelope, traveling in one direction, multiplied by a plane wave traveling in the opposite direction. The FWMs have the appealing features that they undergo only local variations, they do not spread out as they propagate in free space, and they travel with the speed of light in straight lines. The vector FWMs were derived by Brittingham[1] in a heuristic way. More motivated derivations were carried out by Sezginer,[2] Belanger,[3] and Ziolkowski[4] who obtained FWM solutions to the scalar wave equation and used them as Hertzian potentials to determine the corresponding vector solutions to Maxwell's equations. Although the FWMs have an infinite total energy content, they still have a finite energy density, a property they share with sinusoidal plane-wave solutions.

The popular use of plane waves to represent moving particles defies our intuitive notion of particles as localized solutions to field equations. Other, localized solutions, e.g., Gaussian pulses, tend to spread out as they propagate in free space. In contradistinction, the FWM solutions have the attractive property of staying localized for all time; as a consequence, they are more suitable for representing light particles (photons). The importance of this property is quite clear in view of the fact that particle localization is the only phenomenon that links us to the microphysical world. For example, a track left by a particle in a cloud chamber or a dot left by a photon on a photographic plate are just manifestations of the localization of particles, a concept that has been undermined in the current interpretation of quantum mechanics.

These ideas concerning particle localization are not completely new; they reflect a position that was advocated by Einstein and de Broglie,[5,6] among others. In their view, a particle is perceived as a high concentration of a field governed by a partial differential equation, e.g., Maxwell's equations, the Klein–Gordon equation, etc. This highly concentrated field, or "bunch field," must remain localized and must not spread out as the particle travels in space-time. In this picture, the bunch field is incorporated in an extended wave field, thus combining the wave and the corpuscular aspects of matter. As in the case of massless particles, this interpretation of the wave-particle duality should be contrasted with Bohr's complementarity principle, whereby a particle manifests itself either in the form of a wave or in the form of a corpuscle, with both characters never being observed simultaneously.

If the idea of the bunch field is adopted, a representation of a particle in the form of a wave packet is one possibility. Until recently, however, it was believed that linear field equations cannot support continuous nonsingular wave packets that do not spread in free motion. (This is not the case for the massless FWMs and the massive nondispersive wave packets derived by MacKinnon.[7,8]) The other possibility is to use a "singularity solution" for representing the physical reality of a localized particle. Such a singular solution to a linear field equation is an approximation to a more general solution of a corresponding nonlinear equation. The nonlinearity has a larger effect near the vicinity of the singularity, where it keeps the field amplitude large but finite. One of the first attempts to incorporate such ideas was de Broglie's in connection with his theory of the "double solution."[9] Other attempts include Madelung's hydrodynamical model[10] and de Broglie's "pilot wave" theory,[9] both of which inspired Bohm[11,12] to develop the idea of the quantum po-

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tential and to use it to give a causal interpretation of quantum mechanics. A common feature of these theories is that the particle kinematics can be derived from the information incorporated in the phase of a quantum mechanical wave function $\Psi = |\Psi| e^{i\phi}$, where both $|\Psi|$ and ϕ are real and the velocity of the particle can be given as

$$u = (1/m)\nabla\phi, \tag{1}$$

a relationship known as the "guidance formula."[9] More recent developments, along the same lines, include the introduction of solitons into field theories,[13] through the study of fields modeled by nonlinear equations, e.g., the cubic Schrödinger equation, the cubic Klein–Gordon equation, the sine-Gordon equation, etc. A rather broad class of such equations has been proposed for modeling localized particles. It is not very clear, however, whether a unique set of equations could be agreed upon to represent massive particles.

It is our purpose in this exposition to investigate the possibility of using Brittingham-like linear structures to represent massive particles. There are two options that we would like to examine. The first one is to think of these nondispersive wave packets as classical billiard-like solutions. In this case the velocity of the particle is the same as the velocity of the wave packet's envelope. The other choice is to follow de Broglie and consider such solutions as quantum mechanical objects whose kinematics can be derived from their phases as in Eq. (1). Since the original FWMs are solutions to the scalar wave equation or Maxwell's equations, they represent massless particles and their envelopes travel in free space with the speed of light. In the case of a massive particle, one should find for the Klein–Gordon equation or the Dirac equation solutions analogous to the FWMs, but with their envelopes traveling at some group velocity v_g smaller than the speed of light c. A previous attempt[14] was made to find localized solutions to the Klein–Gordon equation. These solutions were approximate, with an envelope moving at a group velocity v_g very close to the speed of light c, or exact ones with an envelope traveling at the speed of light, a feature that makes them physically unattractive. A Brittingham-like solution to the massive Dirac equation has never been published before. However, Brittingham-like solutions to the massless Dirac equation and the spinor wave equation have been derived by Hillion.[15,16] Again, all these solutions have dealt with massless fields and, consequently, they have envelopes that move in straight lines with the speed of light. It is our aim in this paper to introduce a method for obtaining Brittingham-like solutions to massive fields, in particular, the massive scalar field modeled by the Klein–Gordon equation and the massive spinor field modeled by the Dirac equation. The work is based on an embedding technique that has been utilized to derive a natural basis for the synthesis of Brittingham-like solutions. This novel basis has been termed the bidirectional representation[17] because it is a superposition of elementary solutions built up of a product of two plane waves, one traveling to the left and the other to the right. Our plan is to give a brief introduction to the bidirectional representation in the next section and use it to derive the scalar FWMs. This method will be applied to the Klein–Gordon equation in Sec. III, where solutions analogous to the FWMs, but moving with a group velocity v_g, will be derived. It will be shown that a special case of such solutions is the nondispersive wave packet derived by MacKinnon.[7,8] A comparison of MacKinnon's work to ours will be carried out in Sec. IV. Nondispersive localized solutions to the Dirac equation will be derived in Sec. V and a general discussion of the results will be given in Sec. VI.

II. THE BIDIRECTIONAL REPRESENTATION

The bidirectional representation[17] was originally developed in order to provide a natural basis for synthesizing Brittingham-like solutions. In this section, we shall outline the salient features of this technique and use it to derive the scalar FWMs.

Consider the general equation

$$[\partial_t^2 + \hat{\Omega}(-i\nabla)]\Psi(\mathbf{r},t) = 0, \quad \mathbf{r}\in R^3, \quad t>0, \tag{2}$$

where $\hat{\Omega}(-i\nabla)$ is a positive, self-adjoint, possibly pseudo-differential operator, which can be decomposed as follows:

$$\hat{\Omega}(-i\nabla) = \hat{A}(-i\partial_z) + [\hat{\Omega}(-i\nabla) - \hat{A}(-i\partial_z)]$$

$$\equiv \hat{A}(-i\partial_z) + \hat{B}(-i\nabla_T, -i\partial_z). \tag{3}$$

The manner in which the operators $\hat{A}(-i\partial_z)$ and $\hat{B}(-i\nabla_T, -i\nabla_z)$ are chosen provides a great deal of flexibility; the operator $\hat{A}(-i\partial_z)$ may or may not be a natural part of $\hat{\Omega}(-i\nabla)$ and the choice of the preferred variable z is arbitrary. A splitting of the type given in (3) changes Eq. (2) to the form

$$\partial_t^2\Psi(\mathbf{r},t) + \hat{A}(-i\partial_z)\Psi(\mathbf{r},t) + \hat{B}(-i\nabla_T, -i\partial_z)\Psi(\mathbf{r},t) = 0. \tag{4}$$

We introduce, next, the Fourier transform with respect to the transverse (with respect to z) variables, viz.,

$$\Psi(\mathbf{r},t) = \frac{1}{(2\pi)^2}\int_{R^2} d\boldsymbol{\kappa}\, \tilde{\psi}(\boldsymbol{\kappa},z,t) e^{-i\boldsymbol{\kappa}\cdot\rho}. \tag{5}$$

The spectrum $\tilde{\psi}(\boldsymbol{\kappa},z,t)$ is governed by the equation

$$\partial_t^2\tilde{\psi}(\boldsymbol{\kappa},z,t) + \hat{A}(-i\partial_z)\tilde{\psi}(\boldsymbol{\kappa},z,t) + \hat{B}(-\boldsymbol{\kappa}, -i\partial_z)\tilde{\psi}(\boldsymbol{\kappa},z,t) = 0. \tag{6}$$

In terms of new variables

$$\zeta = z - t\,\mathrm{sgn}(\alpha)\alpha^{-1}A^{1/2}(\alpha), \tag{7a}$$

$$\eta = z + t\,\mathrm{sgn}(\beta)\beta^{-1}A^{1/2}(\beta), \tag{7b}$$

an elementary solution to Eq. (6) is given by

$$\psi_e(z,t,\beta,\alpha) = e^{-i\alpha\zeta(\beta,\alpha)}e^{+i\beta\eta(\beta,\alpha)}, \tag{8}$$

provided that the following constraint is satisfied:

$$-[A(\alpha) + A(\beta) + 2\,\mathrm{sgn}(\alpha)A^{1/2}(\alpha)\,\mathrm{sgn}(\beta)A^{1/2}(\beta) - A(\beta-\alpha)] + B(\boldsymbol{\kappa},(\beta-\alpha)) \equiv K(\alpha,\beta,\boldsymbol{\kappa}) = 0. \tag{9}$$

The elementary solution given in Eq. (8) consists of a product of two plane waves traveling in opposite directions, with wave-number-dependent phase speeds equal to $\mathrm{sgn}(\alpha)\alpha^{-1}A^{1/2}(\alpha)$ and $\mathrm{sgn}(\beta)\beta^{-1}A^{1/2}(\beta)$, respectively. A general solution to Eq. (2) can be constructed from the

elementary solutions of the type given in (8) by a linear superposition; specifically,

$$\Psi(\mathbf{r},t)=\frac{1}{(2\pi)^2}\int_{R^2}d\boldsymbol{\kappa}\,e^{i\boldsymbol{\kappa}\cdot\boldsymbol{\rho}}\int_{R^1}d\alpha\int_{R^1}d\beta\,C(\alpha,\beta,\boldsymbol{\kappa})$$
$$\times e^{+i\alpha\zeta(\alpha,z,t)}e^{-i\beta\eta(\beta,z,t)}\delta[K(\alpha,\beta,\boldsymbol{\kappa})]. \tag{10}$$

A detailed analysis of this representation and its relation to a Fourier superposition can be found in Ref. 17, where it was applied to various classes of equations, e.g., the 3-D scalar wave equation, the 3-D Klein–Gordon equation, and the telegraph equation. As mentioned earlier, the resulting solutions had envelopes moving with the speed of light, a property we would like to avoid in the next section.

As an example, we shall apply the bidirectional representation to the 3-D scalar wave equation, viz.,

$$\partial_t^2\Psi(\mathbf{r},t)-c^2\nabla^2\Psi(\mathbf{r},t)=0, \tag{11}$$

where $\hat{\Omega}(-i\nabla)$ is now defined as

$$\hat{\Omega}(-i\nabla)=-c^2\nabla^2. \tag{12}$$

We can choose the $\hat{A}(-i\partial_z)$ and $\hat{B}(-i\nabla_T,-i\partial_z)$ operators as follows:

$$\hat{A}(-i\partial_z)=-c^2\partial_z^2, \tag{13a}$$

$$\hat{B}(-i\nabla_T,-i\partial_z)=-c^2\nabla_T^2. \tag{13b}$$

This decomposition results in the characteristic variables

$$\zeta=z-ct \quad\text{and}\quad \eta=z+ct, \tag{14}$$

and the constraint relationship

$$K(\alpha,\beta,\boldsymbol{\kappa})\equiv-4\alpha\beta+\kappa^2=0. \tag{15}$$

Specializing the representation given in Eq. (10), an azimuthally symmetric solution to the scalar wave equation can be written explicitly as

$$\Psi(\mathbf{r},t)$$
$$=\frac{1}{(2\pi)^2}\int_0^\infty d\kappa\,\kappa J_0(\kappa\rho)\int_0^\infty d\beta\int_0^\infty d\alpha\,\delta\left(\alpha\beta-\frac{\kappa^2}{4}\right)$$
$$\times C(\alpha,\beta,\kappa)e^{-i\alpha(z-ct)}e^{i\beta(z+ct)} \tag{16}$$

or

$$\Psi(\mathbf{r},t)=\frac{1}{(2\pi)^2}\int_0^\infty d\kappa\int_0^\infty d\beta\,\frac{\kappa}{\beta}J_0(\kappa\rho)$$
$$\times C\left(\frac{\kappa^2}{4\beta},\beta,\kappa\right)e^{-i\kappa^2/4\beta}e^{i\beta\eta}, \tag{17}$$

upon carrying out the integration over α in Eq. (16).

Let us choose the spectrum

$$C(\kappa^2/4\beta,\beta,\kappa)=(\sqrt{\pi}/2)\sigma e^{-\sigma^2(\beta-\beta')^2}e^{-a_1\kappa^2/4\beta}. \tag{18}$$

Carrying out the integration over κ and β in Eq. (17) and taking the limit as $\sigma\to\infty$, we obtain the zeroth order FWM solution;[17] specifically,

$$\Psi(\mathbf{r},t)=[4\pi(a_1+i\zeta)]^{-1}e^{-\beta'\rho^2/(a_1+i\zeta)}e^{i\beta'\eta}. \tag{19}$$

It has been demonstrated by the authors[17] that for very small values of a_1 this function behaves like a localized pulse that moves in the positive z direction with speed c. Since a_1 is not dimensionless, we can use the more stringent condition $\beta' a_1\ll 1$. A good estimate of the waist of such a pulse is $(a_1/\beta')^{1/2}$; as a consequence, the condition $(a_1/\beta')^{1/2}\ll 1/\beta'$ has to be satisfied. If β' is assumed to be a characteristic wave number, with a corresponding wavelength $\lambda=2\pi/\beta'$, the condition given earlier becomes $(a_1/\beta')^{1/2}\ll\lambda$, and for $\Psi(\mathbf{r},t)$ to represent a localized light pulse, its waist must be much less than the characteristic wavelength of an extended wave structure associated with it. If, on the other hand, $\beta' a_1>1$, the plane-wave term $\exp(i\beta\eta)$ takes over and $\Psi(\mathbf{r},t)$ degenerates into a nonlocalized sinusoidal function traveling in the negative z direction.

Solutions such as the one in Eq. (19) can be very interesting when it comes to modeling the microphysical world; they are characterized, however, by infinite total energies. A superposition of FWMs, suggested by Ziolkowski,[4] yields finite energy, highly localized pulses of unusual decay patterns. These slow energy decay patterns have been confirmed experimentally,[18] and it has been shown that specific pulses, e.g., the modified power spectrum (MPS) pulse,[19] hold together for longer distances than Gaussian pulses.

III. THE KLEIN–GORDON EQUATION

In this section, we shall apply the bidirectional representation to the 3-D Klein–Gordon equation given by

$$\partial_t^2\Psi(\mathbf{r},t)-c^2\nabla^2\Psi(\mathbf{r},t)+\mu^2c^2\Psi(\mathbf{r},t)=0, \tag{20}$$

where $\mu=m_0c/\hbar$, m_0 being the rest mass and $\hbar$ is Planck's constant divided by 2π. A comparison of this equation with (2) shows that

$$\hat{\Omega}(-i\nabla)\equiv-c^2\nabla^2+\mu^2c^2. \tag{21}$$

In our previous work[14] the operator $\hat{\Omega}(-i\nabla)$ was split as follows:

$$\hat{\Omega}(-i\nabla)=\hat{A}(-i\partial_z)+\hat{B}(-i\nabla_T,-i\partial_z), \tag{22}$$

$$\hat{A}(-i\partial_z)=-c^2\partial_z^2, \tag{23a}$$

$$\hat{B}(-i\nabla_T,-i\partial_z)=-c^2\nabla_T^2+\mu^2c^2. \tag{23b}$$

This decomposition led to the characteristic variables

$$\zeta=z-ct,\quad \eta=z+ct, \tag{24}$$

and, upon superposition, to a wave packet with an envelope moving with the speed of light, exactly as in the case of massless particles.

In the following, we propose to split the operator $\hat{\Omega}(-i\nabla)$ in a more physical way so that we can obtain envelopes that move with a group velocity smaller than c; specifically,

$$\hat{\Omega}(-i\nabla)=\hat{A}(-i\partial_z)+\hat{B}(-i\nabla_T,-i\partial_z), \tag{25}$$

$$\hat{A}(-i\partial_z)=-c^2\partial_z^2+\mu^2c^2, \tag{26a}$$

$$\hat{B}(-i\nabla_T,-i\partial_z)=-c^2\nabla_T^2. \tag{26b}$$

This choice of the operators $\hat{A}$ and $\hat{B}$ gives rise to the characteristic variables

$$\zeta=z-ct\,[\mathrm{sgn}(\alpha)/\alpha](\alpha^2+\mu^2)^{1/2}, \tag{27a}$$

$$\eta=z+ct\,[\mathrm{sgn}(\beta)/\beta\,](\beta^2+\mu^2)^{1/2}, \tag{27b}$$

and the constraint relationship

$$K(\alpha,\beta,\kappa)=\kappa^2-[\mu^2+2\alpha\beta+2\,\mathrm{sgn}(\alpha)(\alpha^2+\mu^2)^{1/2}\times\mathrm{sgn}(\beta)(\beta^2+\mu^2)^{1/2}]=0. \tag{28}$$

Following the recipe given in Sec. II, a general solution to Eq. (20) can be written as follows:

$$\Psi(\mathbf{r},t)=\frac{1}{(2\pi)^2}\int_{R^2}d\kappa\, e^{-i\kappa\cdot\rho}\int_{R^1}d\alpha\int_{R^1}d\beta \times C(\alpha,\beta,\kappa)\delta[K(\alpha,\beta,\kappa)] \times\exp[-i\alpha(z-ct\,\mathrm{sgn}(\alpha)(\alpha^2+\mu^2)^{1/2}/\alpha)] \times\exp[i\beta(z+ct\,\mathrm{sgn}(\beta)(\beta^2+\mu^2)^{1/2}/\beta)]. \tag{29}$$

Analogously to the FWMs, we choose the spectrum entering into (29) as

$$C(\alpha,\beta,\kappa)=\bar{C}(\alpha,\kappa)\delta(\beta-\beta_0). \tag{30}$$

It follows, then, that

$$\Psi(\mathbf{r},t)=G(\rho,z,t) \times\exp[i\beta_0(z+ct\,\mathrm{sgn}(\beta_0)(\beta_0^2+\mu^2)^{1/2}/\beta_0)], \tag{31}$$

where

$$G(\rho,z,t)=\frac{1}{(2\pi)^2}\int_{R^2}d\kappa\, e^{i\kappa\cdot\rho}\int_{R^1}d\alpha\,\bar{C}(\alpha,\kappa)\delta[K(\alpha,\beta_0,\kappa)] \times\exp[i\alpha(z-ct\,\mathrm{sgn}(\alpha)(\alpha^2+\mu^2)^{1/2}/\alpha)]. \tag{32}$$

We can find explicit FWM-like solutions to Eq. (20) by choosing a spectrum $\bar{C}(\alpha,\kappa)$ and carrying out the integrations in Eq. (32). This is a very tedious task, however, especially when dealing with a complicated constraint relationship such as the one given in Eq. (28). Alternatively, we can find the differential equation governing $G(\rho,z,t)$ by substituting (31) into the 3-D Klein–Gordon equation. If this procedure is implemented, we obtain

$$i2\beta_0(\partial_z-v_g^{-1}\partial_t)G(\rho,z,t)+(\partial_z^2-c^{-2}\partial_t^2) \times G(\rho,z,t)+\nabla_T^2G(\rho,z,t)=0, \tag{33}$$

where v_g is a group velocity given by

$$v_g=c\beta_0/\mathrm{sgn}(\beta_0)(\beta_0^2+\mu^2)^{1/2}. \tag{34}$$

It should be noted that v_g can be derived by differentiating the angular frequency characterizing the left-going plane wave with respect to the wave number β_0.

Motivated by the ansatz leading to the FWMs in the case of the scalar wave equation and by the existence of the convection term $(\partial_z-v_g^{-1}\partial_t)G(\rho,z,t)$ in Eq. (33), we seek solutions of the form

$$G(\rho,z,t)\equiv G(\rho,\tau), \tag{35a}$$

$$\tau=\gamma(z-v_gt), \tag{35b}$$

$$\gamma=(1-v_g^2/c^2)^{-1/2}. \tag{35c}$$

Equation (33) becomes, then, a hyperbolized Schrödinger-like equation, viz.,

$$i4\beta_0\gamma\partial_\tau G(\rho,\tau)+\partial_\tau^2G(\rho,\tau)+\nabla_T^2G(\rho,\tau)=0. \tag{36}$$

It is now clear that v_g is the group velocity associated with a classical billiard-like particle represented by the enveloped of $G(\rho,\tau)$. In our previous work,[14] we obtained solutions to (36) for $\gamma\gg1$, or, equivalently, for $v_g\simeq c$. To obtain an exact solution to Eq. (36), we express $G(\rho,\tau)$ in the form

$$G(\rho,\tau)=g(\rho,\tau)e^{-i2\beta_0\gamma\tau}. \tag{37}$$

A substitution of (37) into (36) results in the Helmholtz equation:

$$\nabla_T^2g(\rho,\tau)+\partial_\tau^2g(\rho,\tau)+4\beta_0^2\gamma^2g(\rho,\tau)=0. \tag{38}$$

The steps leading to (38) are interesting by themselves since they reduce the 3-D Klein–Gordon equation, which is hyperbolic, to a 3-D Helmholtz equation, which is elliptic. More importantly, however, a solution to Eq. (38) represents an envelope that travels with a velocity v_g and retains its shape for all time. As a consequence, a large class of exact nondispersive solutions to the 3-D Klein–Gordon equation can be derived from exact solutions to the Helmholtz equation. One possible solution can be expressed in terms of the spherical Bessel functions, viz.,

$$g(\rho,\tau)=j_l(2\beta_0\gamma R)P_l^m(\tau/R)\cos(m\phi),$$

where $R=\sqrt{\rho^2+\tau^2}$, j_l is the spherical Bessel function of order l and P_l^m is the associated Legendre function. Now, exact solutions to the Klein–Gordon equation can be written as follows:

$$\Psi_{lm}(\mathbf{r},t)=j_l(2\beta_0\gamma R)P_l^m(\tau/R) \times\cos(m\phi)e^{-i2\beta_0\gamma\tau}e^{i\beta_0\eta}. \tag{39}$$

For azimuthally symmetric solutions ($m=0$), the zeroth order mode is given by

$$\Psi_{00}(\mathbf{r},t)=j_0(2\beta_0\gamma R)e^{-i2\beta_0\gamma\tau}e^{i\beta_0\eta}. \tag{40}$$

Its amplitude decreases as ρ^{-1} in the transverse direction and as τ^{-1} in the direction of propagation. This is a property shared by all even modes ($l=$ even integer). On the other hand, odd modes are more localized in the transverse direction. To see this, consider the first-order mode, viz.,

$$\Psi_{01}(\mathbf{r},t)=j_1(2\beta_0\gamma R)(\tau/R)e^{-i2\beta_0\gamma\tau}e^{i\beta_0\eta}. \tag{41}$$

For large arguments, $j_1(z)\simeq\sin(z-\pi/2)/z$; consequently, $\Psi_{01}(\mathbf{r},t)$ decays as ρ^{-2} in the transverse direction, but still decays as τ^{-1} in the z direction. These decay properties indicate that the solutions given in Eq. (39) have infinite total energy content, a feature they share with plane-wave solutions and Brittingham's FWMs. In analogy to the FWMs, localized slowly decaying solutions to the Klein–Gordon equation, with a finite energy content, can be synthesized as a superposition of the wave packets given in Eq. (39).

As long as $\Psi(\mathbf{r},t)$ is treated as a classical field, the kinematics of a particle represented by it can be derived from the energy and the momentum densities of a Klein–Gordon field, viz.,

$$H(\mathbf{r},t)=c^{-2}\partial_t\Psi(\mathbf{r},t)\partial_t\Psi^*(\mathbf{r},t)+\nabla\Psi(\mathbf{r},t)\cdot\nabla\Psi^*(\mathbf{r},t)+\mu^2\Psi(\mathbf{r},t)\Psi^*(\mathbf{r},t),$$

$$\mathbf{P}(\mathbf{r},t)=-c^{-2}[\partial_t\Psi(\mathbf{r},t)\nabla\Psi^*(\mathbf{r},t)+\partial_t\Psi^*(\mathbf{r},t)\nabla\Psi(\mathbf{r},t)].$$

As mentioned earlier, solutions of infinite energy content, such as those given in Eq. (39), can be superimposed to obtain finite energy ones. In this case, the integration of $H(\mathbf{r},t)$ and $\mathbf{P}(\mathbf{r},t)$ over all space will give the energy and the momentum of the particle represented by such solutions. Another possibility is to search for nondispersive bump solutions of finite energy densities. For a solution of this kind the central portion of the field has a larger energy content and small oscillations compared to the tails. The relatively large oscillations of the tails cancel out on the average when such a field interacts with a large scale measuring instrument. Space will appear to be empty except for the large amplitude, oscillation-free central portion. In this case, the energy and the momentum of the particle can be calculated by integrating the energy and momentum densities over the central part of the field. A crude example of what we mean is the integration of the one-dimensional function $\sin(x)/x$ over all values of x from $-\infty$ to $+\infty$. This will give a value of π which is approximately equal to the area under the first lobe of the function between its first two zeroes. In an interaction of such a field with another bump field (e.g., the FWM pulse), the interaction will be very large when the central parts of both fields overlap; at the same time the tails will be averaged out. In such a case the large amplitude central portions of the fields are the only parts that really contribute to the interaction and can be measured. An interaction theory is needed to provide a more rigorous and complete discussion of this possibility; the development of such a theory is out of the scope of this work.

Solutions describing nondispersive wave packets are not restricted to the form given in Eq. (39); as mentioned earlier, any solution to Eq. (36) will give a wave packet that will keep its form as it travels in free space. A special case of these solutions has been derived by MacKinnon,[7,8] who demonstrated that a de Broglie wave packet can be formed by assuming that the phase of a particle's internal vibration is independent of the choice of a reference frame. MacKinnon's solution is almost identical to the Ψ_{00} mode, especially when the terms in the exponent are rearranged so that

$$\Psi_{00}(\mathbf{r},t) = j_0(2\beta_0\gamma R)e^{-i\beta_0\gamma^2(1+v_g^2/c^2)[z-(c^2/v_g)t]}. \tag{42}$$

Because of the close resemblance of the two solutions, it is of interest to compare more closely the methods leading to them. This comparison will be carried out in the next section, where the difference between the interpretations of the solution in (39) as a classical wave function and as a quantum mechanical wave packet will be investigated. A discussion will also be provided of the dispersion relationships involved and their effect on the kinematics of a free particle represented by a wave packet such as the one in Eq. (42).

Before we proceed to the next section, it is worthwhile to point out that the de Broglie relationship between the group velocity v_g of the envelope and the phase velocity $v_{\rm ph}$ of the associated plane wave (i.e., $v_{\rm ph}v_g = c^2$) is embodied automatically in Eq. (42) by simply imposing the requirement that $\Psi(\mathbf{r},t)$ should be a nonsingular continuous wave packet that does not disperse with time. It is quite interesting that the localization requirement alone can lead to such a relationship, without any reference to an "internal clock" of the particle, or the need for the assumption that the phase of the internal clock of the particle be equal to the phase of the associated wave, two concepts utilized by de Broglie to derive the relationship $v_{\rm ph}v_g = c^2$ in his attempt to maintain the invariance of the relationship $mc^2 = h\nu$ for all frames of reference. The particle-wave velocity equation $v_{\rm ph}v_g = c^2$ has been considered[20] to be a generalization of the more limited velocity relation $v_g = v_{\rm ph} = c^2$, which is true for massless particles only. Moreover, it has been argued by MacGregor[20] that the relationship $v_{\rm ph}v_g = c^2$ should be taken as a basic postulate of special relativity, replacing the popular postulate that the speed of light in free space has the value c in all inertial frames.

IV. NONDISPERSIVE WAVE PACKETS AND DISPERSION RELATIONSHIPS

The similarity between MacKinnon's solution and the Ψ_{00} mode is very clear when we recall that $j_0(x) = \sin(x)/x$. In order to examine these two results more carefully, we first write MacKinnon's 3-D wave packet[8] as

$$\Psi_M(\mathbf{r},t) = [\sin(kR)/kR\,]e^{i[\omega(k_0)t - k_0 z]}, \tag{43}$$

where

$$k = \mu, \tag{44}$$

$$R = \sqrt{\rho^2 + \gamma^2(z-ut)^2}. \tag{45}$$

The parameter k_0 was defined by MacKinnon in the case of the 1-D solution[7] as

$$k_0 = \gamma\mu(u/c). \tag{46}$$

In the 3-D case, it is only correct up to a numerical factor of $\sqrt{2}$, as will be shown later. The frequency $\omega(k_0)$ entering into Eq. (43) was defined as

$$\omega(k_1) - \omega(k_0) = u(k_1 - k_0), \tag{47}$$

with the provision that

$$\partial_{k_0}\omega(k_0) = u \text{ and } \partial^2_{k_0}\omega(k_0) = 0. \tag{48}$$

These conditions were claimed by MacKinnon to be necessary for the wave packet to retain its form for all time. The velocity u of the particle is derived from the derivative of $\omega(k_0)$ with respect to k_0. However, the explicit dependence of $\omega(k_0)$ on k_0 is not very obvious, and the adequacy of the definition given by (47) is questionable.

Our aim in this section is to clarify these issues through a detailed analysis of the properties of the solutions given in Eqs. (42) and (43). The main difference between the two solutions is that Ψ_{00} has been treated, until now, as a classical nondispersive wave packet with an envelope that moves with a velocity v_g defined in Eq. (34). This is not, however, a unique velocity as will be shown in this section. The wave function Ψ_M, on the other hand, is considered to be a quantum mechanical entity moving with a velocity u derived from a dispersion relationship as in Eq. (48). In order to compare the two wave functions, we will consider Ψ_{00}, for the rest of this section, to be a quantum mechanical wave packet. In this case, the group velocity v_g might not be consistent with the fact that the kinematics of a particle should

be derived from its phase factor. To check such an inconsistency we can refer to the particle's energy and momentum relationships. As stated earlier, the energy and the momentum can be calculated by taking the derivatives of the phase of Ψ_{00} with respect to time and space, respectively, viz.,

$$E = \hbar\partial_t\phi, \quad p = -\hbar\nabla\phi. \tag{49}$$

Using $\Psi_{00}(\mathbf{r},t)$ in Eq. (42) together with definition of v_g given by Eq. (34), we obtain the following expressions for the energy and the z component of the momentum:

$$E = \frac{c^2}{[1-v_g^2/c^2]^{1/2}} m_0 \frac{[1+v_g^2/c^2]}{[1-v_g^2/c^2]}, \tag{50a}$$

$$P_z = \frac{v_g}{[1-v_g^2/c^2]^{1/2}} m_0 \frac{[1+v_g^2/c^2]}{[1-v_g^2/c^2]}. \tag{50b}$$

These are incorrect expressions unless we use an apparent rest mass

$$M_0 = m_0 \frac{[1+v_g^2/c^2]}{[1-v_g^2/c^2]}, \tag{51}$$

which is identical to the "apparent mass" introduced by de Broglie[9] in order to guarantee the consistency of the equations of motion of particles represented by such wave packets. The apparent mass is defined as

$$M_0 = \sqrt{m_0^2 + \delta m_0^2}, \tag{52a}$$

$$\delta m_0^2 = (\hbar^2/c^2)(1/\psi)(c^{-2}\partial_t^2 - \nabla^2)\psi. \tag{52b}$$

The quantity ψ in Eq. (52b) is defined through the relationship $\Psi(\mathbf{r},t) = \psi[R(\mathbf{r},t)]f(z,t)$. To arrive at the definition of M_0 given in (52), one should take into account that $R = \sqrt{\rho^2 + \gamma^2(z-v_g t)^2}$ and that β_0 is related to v_g through Eq. (34), from which one has $\beta_0^2 = \mu^2(v_g^2/c^2)/(1-v_g^2/c^2)$.

The redefinition of the mass M_0, as given in (51), produces the expected energy and momentum relations. The results are physically unattractive, however, because of the dependence of M_0 on v_g. On the other hand, MacKinnon[8] has indicated that his solution cannot suffer from such a problem because, for $|\psi| = \sin(\psi R)/\psi R$, it follows that $\delta m_0 = \mu\hbar/c$ and the apparent mass reduces to

$$M_0 = \sqrt{2}m_0. \tag{53}$$

To overcome the difficulty associated with the solution $\Psi_{00}(\mathbf{r},t)$ obtained by utilizing the bidirectional representation, we can start with the ansatz

$$\Psi(\mathbf{r},t) = G(\boldsymbol{\rho},z,t)e^{i\beta_0(z+(c^2/u)t)}, \tag{54}$$

where, now, the particle velocity, designated by u, is left undefined. Substitution of (54) into Eq. (20) gives a generalization of the partial differential Eq. (33), viz.,

$$i2\beta_0(\partial_z - u^{-1}\partial_t)G(\boldsymbol{\rho},z,t) + (\partial_z^2 - c^{-2}\partial_t^2)G(\boldsymbol{\rho},z,t) + \nabla_T^2 G(\boldsymbol{\rho},z,t) + (\beta_0^2\gamma^{-2}(c^2/u^2) - \mu^2)G(\boldsymbol{\rho},z,t) = 0, \tag{55}$$

where

$$\gamma = (1-u^2/c^2)^{-1/2}.$$

Motivated by the convection term on the left-hand side of Eq. (55), we can choose

$$G(\boldsymbol{\rho},z,t) = g(\boldsymbol{\rho},\tau)e^{-i2\beta_0\gamma\tau}, \quad \tau = \gamma(z-ut), \tag{56}$$

which reduces (55) into a Helmholtz equation; specifically,

$$\nabla_T^2 g(\boldsymbol{\rho},\tau) + \partial_\tau^2 g(\boldsymbol{\rho},\tau) + \chi^2 g(\boldsymbol{\rho},\tau) = 0, \tag{57a}$$

$$\chi^2 = 4\beta_0^2\gamma^2 + (\beta_0^2/\gamma^2)(c^2/u^2) - \mu^2. \tag{57b}$$

A solution to the Klein–Gordon equation can be written now as follows:

$$\Psi(\mathbf{r},t) = [\sin(\chi R)/\chi R] \times \exp[i\beta_0(1+u^2/c^2)\gamma^2(z-(c^2/u)t)]. \tag{58}$$

It should be noted that χ is identical to MacKinnon's k. The value of $u = u(\beta_0)$ can be deduced from the algebraic relationship (57b). Instead, we introduce the change of variables

$$k_0 = \beta_0\gamma^2(1+u^2/c^2), \tag{59}$$

which yields, upon substitution into Eq. (57b), the following expression for the velocity:

$$u = \pm ck_0/\sqrt{k_0^2 + \chi^2 + \mu^2}. \tag{60}$$

In the case of MacKinnon's wave packet, u was treated as a parameter independent of k_0. However, such an assumption does not make sense because the relationship $p_z = \hbar k_0$ for the momentum implies that p_z depends on k_0, and one expects the velocity to change as the momentum varies.

The definition of k_0 given in (59) changes the wave packet into the form

$$\Psi(\mathbf{r},t) = [\sin(\chi R)/\chi R]e^{i(\omega(k_0)t - k_0 z)}, \tag{61}$$

where

$$\omega(k_0) = (c^2/u)k_0. \tag{62}$$

An explicit dispersion relationship for $\omega(k_0)$ can be found by combining Eqs. (60) and (62); specifically,

$$\omega(k_0) = \pm c\sqrt{k_0^2 + \chi^2 + \mu^2}. \tag{63}$$

The positive and negative signs correspond to positive and negative energies, respectively. It is tempting to think of χ and k_0 as transverse and longitudinal wave numbers, respectively. This is not the case, however, and for the wave packet to represent a quantum mechanical particle moving in free space, we need to introduce the notion of an apparent mass M_0, as defined in Eq. (52). It is straightforward to show that $M_0 = (\chi^2 + \mu^2)^{1/2}\hbar/c$, and using Eq. (63) we arrive at the familiar energy momentum relationship

$$E = \pm c\sqrt{p^2 + M_0^2 c^2}, \tag{64}$$

where we have made use of the relationships $p = \hbar k_0$ and $E = \hbar\omega(k_0)$.

If we choose $\chi = \mu$, the velocity relationship reduces to

$$u = ck_0/\sqrt{k_0^2 + 2\mu^2}, \tag{65}$$

which resembles the group velocity of a 1-D wave packet with an apparent mass $M_0 = \sqrt{2}\mu\hbar/c$. Furthermore, using Eq. (65), an expression for k_0 can be easily derived, viz.,

$$k_0 = \sqrt{2}\gamma\mu(u/c), \tag{66}$$

which is the correct definition of k_0 for the 3-D wave packet.

It should be pointed out that the velocity expression given in Eq. (60) satisfies neither (47) nor the second provision in Eq. (48), i.e., the conditions claimed by MacKinnon as necessary for the construction of nondispersive wave packets. The similarity between the definitions of u and v_g should, also, be noted. Beside the factor of $\sqrt{2}$, which appears in the apparent mass, i.e., $\mu^2 \to 2\mu^2 = (M_0/\hbar c)^2$, the main difference between the expressions (34) and (65) is that β_0 is replaced by k_0. The velocity u, on the other hand, leads to the correct kinematics only because the momentum and energy operators are specified as in Eq. (49). If these operators are defined differently, we need a velocity different from u to get the correct kinematics.

It can be deduced from the comparison carried out in this section that the velocity u and the wave numbers β_0 or k_0 enter as parameters that can be defined freely within the limits set up by the dispersion condition (57b). The transformation (59) was introduced in order to demonstrate that one can arrive at MacKinnon's solution as a special case for the choice of u and β_0. It is very important to emphasize this freedom and to point out that different choices can lead to various kinematics depending on the manner in which the quantum mechanical operators are specified.

V. THE DIRAC EQUATION

The exposition given in Sec. II might give one the impression that the bidirectional representation is only applicable to second-order equations that are quadratic in the time derivative. This is not the case, since it can be applied to the Schrödinger equation as well as the Dirac equation. In this section, the de Broglie wave packet derived in the case of a scalar Klein–Gordon field will be used to find nondispersive wave packets for the vector fields representing massive spin 1/2 fermions. Such particles are naturally represented by the Dirac equation. It is well known, however, that fermions can be represented rather satisfactorily by a spinorial form of the Klein–Gordon equation.[21]

We begin with the second-order equation:

$$(ic^{-1}\partial_t + \boldsymbol{\sigma}\cdot\nabla)(ic^{-1}\partial_t - \boldsymbol{\sigma}\cdot\nabla)\phi(\mathbf{r},t) = \mu^2\phi(\mathbf{r},t), \tag{67}$$

where $\boldsymbol{\sigma}$ are Pauli matrices, viz.,

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{68}$$

and $\phi(\mathbf{r},t)$ is a two-component spinor. Making use of the properties of the Pauli matrices it can be shown that Eq. (67) can be reduced to the two-component spinorial Klein–Gordon equation:

$$(c^{-2}\partial_t^2 - \nabla^2)\phi(\mathbf{r},t) + \mu^2\phi(\mathbf{r},t) = 0. \tag{69}$$

To find a nondispersive packet solution representing a massive spin 1/2 field, we can choose a solution to Eq. (69) similar to that given in Eq. (61); namely,

$$\phi(\mathbf{r},t) = \begin{bmatrix} \phi_a \\ \phi_b \end{bmatrix} j_0(\chi R) e^{i(\omega(k_0)t - k_0 z)}. \tag{70}$$

This spinor field can be used to derive solutions to the Dirac equation:

$$\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \mu\right)\Psi_D(\mathbf{r},t) = 0, \tag{71}$$

The definitions of the gamma matrices entering into this equation are given in Ref. 21; $\Psi_D(\mathbf{r},t)$ is a four-component spinor defined as follows:

$$\Psi_D(\mathbf{r},t) = \begin{bmatrix} \phi^R(\mathbf{r},t) + \phi^L(\mathbf{r},t) \\ \phi^R(\mathbf{r},t) - \phi^L(\mathbf{r},t) \end{bmatrix}. \tag{72}$$

The two-component spinors $\phi^L(\mathbf{r},t)$ and $\phi^R(\mathbf{r},t)$ are related to $\phi(\mathbf{r},t)$ given in Eq. (70) as follows:

$$\phi^L(\mathbf{r},t) = \phi(\mathbf{r},t), \tag{73a}$$

$$\phi^R(\mathbf{r},t) = (i/\mu)(c^{-1}\partial_t - \boldsymbol{\sigma}\cdot\nabla)\phi(\mathbf{r},t). \tag{73b}$$

Carrying out the operations indicated in (73b), we find that

$$\Psi_D(\mathbf{r},t) = \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} e^{i(\omega t - k_0 z)}, \tag{74}$$

where

$$\psi_1 = \phi_a\left\{i\left(1 + \frac{u}{c}\right)\chi j_1(\chi R)\gamma^2\frac{(z-ut)}{\mu R} + \left(1 - \frac{\omega}{\mu c} - \frac{k_0}{\mu}\right)j_0(\chi R)\right\} + i\phi_b\chi j_1(\chi R)\frac{(x-iy)}{\mu R}, \tag{74a}$$

$$\psi_2 = i\phi_a\chi j_1(\chi R)\frac{(x+iy)}{\mu R} - \phi_b\left\{i\left(1 - \frac{u}{c}\right)\chi \times j_1(\chi R)\gamma^2\frac{(z-ut)}{\mu R} - \left(1 - \frac{\omega}{\mu c} + \frac{\kappa_0}{\mu}\right)j_0(\chi R)\right\}, \tag{74b}$$

$$\psi_3 = \phi_a\left\{i\left(1 + \frac{u}{c}\right)\chi j_1(\chi R)\gamma^2\frac{(z-ut)}{\mu R} \times -\left(1 + \frac{\omega}{\mu c} + \frac{k_0}{\mu}\right)j_0(\chi R)\right\} + i\phi_b\chi j_1(\chi R)\frac{(x-iy)}{\mu R}, \tag{74c}$$

$$\psi_4 = i\phi_a\chi j_1(\chi R)\frac{(x+iy)}{\mu R} - \phi_b\left\{i\left(1 - \frac{u}{c}\right)\chi \times j_1(\chi R)\gamma^2\frac{(z-ut)}{\mu R} + \left(1 + \frac{\omega}{\mu c} - \frac{k_0}{\mu}\right)j_0(\chi R)\right\}. \tag{74d}$$

The four independent solutions to the Dirac equation can be directly obtained from Eq. (74) using the negative and positive energy values of $\omega(k_0)$, in addition to choosing ϕ_a and ϕ_b so that two independent solutions for $\phi(\mathbf{r},t)$ can be obtained, e.g., $\phi_a = 0, \phi_b = 1$ and $\phi_a = 1, \phi_b = 0$. These solutions seem to be quite complicated; nevertheless, they represent a field peaked around the origin that travels in a straight line in free space and does not disperse for all time. Despite the complicated form of the solutions, still some physical results can be obtained. For example, the four independent solutions given in Eqs. (74) are not eigenspinors of the helicity operator Σ_z defined as

$$\Sigma_z = \begin{bmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{bmatrix}. \tag{75}$$

Moreover, if we choose $\phi_a = 1$ and $\phi_b = 0$, the solution given in (74) is still not an eigenstate. We are mainly interested, however, in the large amplitude portion of the field around the center of the pulse ($x = 0, y = 0, z = ut$). In this portion, $j_1(\chi R) \simeq 0$, while $j_0(\chi R) \simeq 1$. Therefore, the components of the spinor given in Eq. (74) can be approximated around the center of the pulse as

$$\psi_1 \simeq 1 - \omega/\mu c - k_0/\mu, \quad \psi_2 \simeq 0,$$
$$\psi_3 \simeq 1 + \omega/\mu c + k_0/\mu, \quad \psi_4 \simeq 0,$$

and $\Psi_D(\mathbf{r},t)$ becomes an eigenspinor of the helicity operator with an eigenvalue $+1$. The same argument can be repeated for $\phi_a = 0$ and $\phi_b = 1$ in order to obtain an eigenspinor with an eigenvalue equal to -1. Similarly, we can get two independent eigenspinors for negative energies with eigenvalues $+1$ and -1.

VI. CONCLUSIONS

The bidirectional representation has been used to derive localized, nondispersive solutions to the Klein–Gordon equation by reducing it to a Helmholtz equation with its z coordinate replaced by the translational variable $\tau = \gamma(z - ut)$. The ansatz leading to such a reduction allows one to derive systematically a large class of nondispersive wave packets, representing massive particles, by making use of the known solutions to the Helmholtz equation. In seeking solutions of this type the particle-wave velocity relationship $v_{\rm ph} v_g = c^2$ follows automatically from the sole requirement of particle localization. The importance of this result need not be emphasized. It is quite intriguing, however, that in order to derive a nondispersive localized solution to the Klein–Gordon equation we arrive at a relationship that guarantees the Lorentz invariance of the formula $h\nu = mc^2$ and which can be used to generalize the postulates of spectial relativity.[20]

A special case of the solutions derived in connection with the Klein–Gordon equation was MacKinnon's nondispersive wave packet. A comparison of this packet to our results helped in clarifying some of the subtleties in MacKinnon's solution; his parameters k, k_0 are now well defined and an explicit form of the dispersion relationship $\omega(k_0)$ has been derived. The derivative of $\omega(k_0)$ with respect to k_0 gives an expression of the velocity which does not satisfy Eq. (47); furthermore, $\omega(k_0)$ is a nonlinear function of k_0, thus violating MacKinnon's condition $\partial^2_{k_0} \omega(k_0) = 0$. The dependence of the velocity on k_0 is expected if one recalls the momentum relationship $p_z = \hbar k_0$; as the momentum of the particle increases, one expects the group velocity of the wave packet representing the particle to increase also.

It has been shown that the apparent mass introduced by de Broglie has to be used in order to obtain the correct energy and momentum describing the motion of massive particles. For the specific wave packet given in Eq. (58) the apparent mass has the value $\hbar c^{-1}(\chi^2 + \mu^2)^{1/2}$. Choosing χ to be proportional to μ through a numerical factor independent of v_g, it follows that M_0 is proportional to the rest mass m_0. On the other hand, if χ is chosen to depend on v_g, the apparent mass M_0 depends on the velocity of the particle, a property which is not very attractive.

The results obtained for the case of the scalar massive Klein–Gordon fields were extended to the spinor massive fields governed by the Dirac equation giving de Broglie nondispersive wave packets representing free massive fermions. This particular application demonstrates that bidirectional solutions can also be derived for field equations characterized by first-order time derivatives. Similar solutions can be obtained for the Schrödinger equation; however, we prefer to publish these results separately because of their relevance to an interesting class of nondispersive solutions to the Schrödinger equation introduced by Berry and Balazs.[22]

In summary, localized, nonsingular, and nondispersive solutions have been derived to linear equations governing the motion of massive particles; specifically, the Klein–Gordon equation and the Dirac equation. Unlike soliton solutions to nonlinear equations, these are solutions to linear equations that can explain the localization properties of particles, at least in free motion. If $\Psi(\mathbf{r},t)$ is treated as a quantum mechanical wave packet, the kinematics of a particle represented by such a field are derived from its phase. On the other hand, if we consider $\Psi(\mathbf{r},t)$ to be a classical field, the kinematics are derived from the energy and momentum densities. A linear superposition can be used to construct finite energy, slowly spreading wave packets. As a consequence, an integration over all space of the field's energy and momentum densities will give the particle's energy and momentum. Another possibility is to derive nonsingular bump field solutions (not neccessarily of finite total energy content) of a large amplitude at the center and much smaller amplitudes but high oscillations at the tails. During an interaction these tails are averaged out and only the central portion of the field can be felt. The kinematics of a particle are, thus, related to the momentum and energy content of the central field. Such localized bump solutions are incorporated in an extended wave field. Using this property, we have been able to justify the wave-particle dualism.[23] We have also been able to provide a novel interpretation of Young's double slit experiment.[24]

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Corepresentations of superalgebras and an antilinear Dirac operator

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The reasons that lead to the use of only linear representations of Lie algebras in quantum theory seem to permit antilinear representations of superalgebras. Such corepresentations of Clifford algebras are investigated and shown to lead to a two-component Dirac equation. It is shown that there exists a one-component corepresentation of the supertranslation algebra, but that this cannot be induced to a corepresentation of the super-Poincaré algebra.

I. INTRODUCTION

According to Wigner's theorem,[1] Appendix to Chap. 20, the symmetries of quantum mechanics should be described by unitary or antiunitary representations of the relevant symmetry group G. Since the squares of both unitary and antiunitary operators are unitary, any element in a Lie group of the form $\exp(tX) = \exp(\frac{1}{2}tX)^2$ must be represented by a unitary operator. This, in turn, means that the elements of the Lie algebra must be represented by linear operators. For superalgebras $g = g_0 \oplus g_1$ there does not appear to be any similar global constraint on the behavior of elements in g_1, opening the possibility that they might be represented by antilinear (conjugate linear) operators. We shall continue to insist that g_0 is to be represented linearly by self-adjoint operators, and this imposes some constraints on the possibilities. If $X \in g_1$ is represented linearly, and $Y \in g_1$ is represented antilinearly then on general grounds the superalgebra bracket $[X,Y]$ must be represented antilinearly. However, since $[X,Y]$ is in g_0 it must be represented linearly, forcing it to vanish. For simplicity we shall examine in detail the simplest case in which the whole of g_1 is represented antilinearly, calling such a linear–antilinear representation of g a *corepresentation*.

In this paper we shall first investigate the corepresentations of Clifford algebras, showing that in some cases these may be of smaller dimension than the ordinary representations. We then apply this to derive an antilinear Dirac operator. Finally, we discuss some corepresentations of the super-Poincaré algebra; we had originally hoped that the use of corepresentations might reduce the size of the supersymmetric multiplets. It turns out that this is true when one considers only the supertranslations but not for a fully super-Poincaré symmetric theory.

II. CLIFFORD ALGEBRAS

Let V be a real vector space with a nonsingular symmetric bilinear form Q, and let

$$g = \mathbf{R} \oplus V$$

be the superalgebra whose only nonzero brackets are

$$[u,v] = 2Q(u,v)$$

with u and v in $g_1 = V$. According to this definition $g_0 = \mathbf{R}$ is central and so must be represented by elements in the center of the commuting (intertwining operator) algebra of any representation.

Lemma 1: Any irreducible corepresentation must map the even part of the center of a superalgebra to real multiples of the identity.

Proof: By the general version of Schur's lemma the intertwining operators for a corepresentation form a real division algebra, so that they must be isomorphic to $\mathbf{R}$, $\mathbf{C}$, or the quaternions $\mathbf{H}$ (compare Ref. 2, Theorem C). The center of $\mathbf{H}$ is $\mathbf{R}$, as is the self-adjoint part of $\mathbf{C}$. (This last comment is not quite obvious, since we know only that the commuting algebra C is isomorphic to $\mathbf{C}$, but do not initially know which elements are self-adjoint. However, by taking the adjoint of the intertwining relation we see that C is invariant under the star (*) operation. Since the star operator is an automorphism over the reals it must act on $C \cong \mathbf{C}$ either as the identity or as complex conjugation. However, if I is the element of C, which corresponds to $i \in \mathbf{C}$, then

$$II = -1 < 0 \leqslant I^*I,$$

so that $I^* \neq I$ and * must act as conjugation. The self-adjoint elements are therefore the real multiples of the identity as asserted.) Since the even part of the center of the superalgebra must be represented by self-adjoint elements of the center of the algebra of intertwining operators the result now follows.

Corollary: Let γ be an irreducible corepresentation of $g = \mathbf{R} \oplus V$. Then γ defines an irreducible linear–antilinear representation of the Clifford algebra of V for a real multiple of Q.

Proof: Since $g_0 = \mathbf{R}$ is represented by real multiples of the identity there must exist a real number λ such that $\gamma(x) = \lambda x$ for all $x \in g_0$. But then the definition of the superalgebra bracket gives

$$[\gamma(u),\gamma(v)]_+ = \gamma([u,v]) = 2\lambda Q(u,v).$$

These are the defining relations for the Clifford algebra of the form λQ, although by definition the operators $\gamma(u)$ and $\gamma(v)$ here are antilinear.

Remark: Unless $\lambda = 0$, in which case the whole theory becomes rather trivial, we can always rescale to obtain $|\lambda| = 1$. Henceforth, we shall assume that this has been done. When $\lambda = 1$ we denote the corresponding Clifford algebra by $C(V,Q)$. For brevity we shall refer to a corepresentation γ of g whose restriction to g_0 is the identity, as a corepresentation of $C(V,Q)$. If $V = \mathbf{R}^{p+q}$ with the pseudo-Euclidean form

$$Q(u,v) = -\sum_{j=1}^{p} u_j v_j + \sum_{j=p+1}^{p+q} u_j v_j$$

we shall write $C^{p,q}$ instead of $C(V,Q)$. To distinguish the

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Minkowski form on space-time when $p = 1$ and $q = 3$ we shall write η instead of Q.

Before proceeding with the general theory we note that the corepresentation theory of Clifford algebras clearly diverges from the representation theory in that there is a one-dimensional corepresentation of the Clifford algebra $C^{0,2}$ whereas its smallest representation is two dimensional. This corepresentation acts on $\mathbf{C}$ by

$$\gamma(u) = \gamma(u_1,u_2) = (u_1 + iu_2)\kappa,$$

where κ denotes the complex conjugation operator. This is because

$$\begin{aligned}\gamma(u)^2 &= (u_1 + iu_2)\kappa(u_1 + iu_2)\kappa \\ &= (u_1 + iu_2)(u_1 - iu_2)\kappa^2 \\ &= (u_1^2 + u_2^2).\end{aligned}$$

Before stating the main theorem of this section we recall that a representation is said to be *real* if there is an antilinear intertwining operator J satisfying $J^2 = 1$, and is said to be *quaternionic* if there is such an antilinear intertwining operator satisfying $J^2 = -1$.

Theorem 1: When $q \geqslant 1$ there is a one–one correspondence between corepresentations of $C^{p,q}$ and real representations of $C^{p,q-1}$. Similarly, when $p \geqslant 1$ there is a one–one correspondence between corepresentations of $C^{p,q}$ and quaternionic representations of $C^{q,p-1}$.

Proof: We shall derive only the second of the two correspondences, as the first follows in a similar but slightly simpler way. Let $e_1, e_2,\ldots,e_{p+q}$ denote the usual basis of $\mathbf{R}^{p+q}$, where $e_1 = (1,0,\ldots,0)$, etc. Given a corepresentation γ of $C^{p,q}$ we set $J = \gamma(e_1)$, and

$$\beta_j = i\gamma(e_{j+1})\gamma(e_1),$$

for $j = 1,\ldots,p+q-1$. It is easy to check that each β_j is linear. Moreover, we have

$$\begin{aligned}[\beta_j,\beta_k]_+ &= -(\gamma(e_{j+1})\gamma(e_1)\gamma(e_{k+1}) \\ &\quad + \gamma(e_{k+1})\gamma(e_1)\gamma(e_{j+1}))\gamma(e_1),\end{aligned}$$

which can be rearranged to give

$$([\gamma(e_{j+1}),\gamma(e_{k+1})]_+)\gamma(e_1)^2 = -2Q(e_{j+1},e_{k+1}),$$

so that the β_j satisfy the relations for a representation of $C^{q,p-1}$. Moreover, J is antilinear, has square

$$\gamma(e_1)^2 = -1,$$

and satisfies

$$J\beta_j = \gamma(e_1)i\gamma(e_{j+1})\gamma(e_1) = i\gamma(e_{j+1})\gamma(e_1)^2 = \beta_j J,$$

so that J defines a quaternionic structure on the representation space. Conversely, given a representation of the Clifford algebra $C^{q,p-1}$ with a quaternionic structure J we may set $\gamma(e_1) = J$ and $\gamma(e_j) = -i\beta_{j-1}J$, for $j > 1$ to get a corepresentation of $C^{p,q}$.

Remark: In general, the irreducible corepresentations of $C^{p,q}$ will correspond to reducible representations of $C^{p,q-1}$ and $C^{q,p-1}$ since the irreducible representations of these lower dimensional Clifford algebras will lack the necessary real or quaternionic structure. In fact, by reference to standard results on the representation theory of Clifford algebras (e.g., Refs. 3 and 4) we arrive at the following conclusions.

Corollary A: The irreducible corepresentations of $C^{p,q}$ correspond to irreducible representations of $C^{p,q-1}$ and $C^{q,p-1}$ if and only if $q - p$ is congruent to 1, 2, or 3 mod 8.

Proof: The irreducible representations of $C^{r,s}$ have a real structure if and only if $s - r \equiv 0,1,2 \bmod 8$, and have a quaternionic structure if and only if $r - s \equiv 2,3,4 \bmod 8$. Thus the irreducibles of $C^{p,q-1}$ have a real structure precisely when $q - p \equiv 1,2,3 \bmod 8$, and the other case follows similarly. (The fact that the two cases yield the same condition on p and q provides a check that no mistake has been made in the calculations.)

Corollary B: The irreducible corepresentations of $C^{p,q}$ have lower dimension than the irreducible representations if and only if $q - p \equiv 2 \bmod 8$.

Proof: The irreducible representations of $C^{p,q-1}$ have lower dimension than those of $C^{p,q}$ if and only if $q + p$ is even, or equivalently $q - p$ is even. Combining this with the previous result yields the stated conclusion. The actual dimension of the irreducible corepresentations is half that of the irreducible representations.

III. THE ANTILINEAR DIRAC OPERATOR

The simplest example of a Clifford algebra satisfying the conditions of Corollary B is $C^{0,2}$, which therefore has a one-dimensional corepresentation. This is, of course, the corepresentation which we gave at the beginning of Sec. II.

The conditions of the corollary also cover the Clifford algebra $C^{1,3}$ associated to Minkowski space, which therefore has a two-dimensional corepresentation. (Actually there are two such corepresentations of opposite helicities corresponding to the two inequivalent irreducible representations of $C^{0,3}$.) Constructing this by the procedures of Theorem 1 we obtain

$$\gamma(v) = \begin{pmatrix} v_2 + iv_1 & i(v_0 - v_3) \\ -i(v_0 + v_3) & v_2 - iv_1 \end{pmatrix}\kappa,$$

where κ is complex conjugation and, to accord with the usual conventions, we have written $v = (v_0,v_1,v_2,v_3)$. It must be noted that the related Clifford algebra $C^{3,1}$ does *not* have such a two-dimensional corepresentation.

One can use this corepresentation to construct an antilinear Dirac operator $D = \gamma(\partial_0,\partial_1,\partial_2,\partial_3)$. In the corresponding two-component Dirac equation

$$D\psi = \mu\psi,$$

the left-hand side is conjugate linear in ψ while the right-hand side is linear, so that the solution space is only a real and not a complex vector space. Nonetheless, applying D a second time yields the Klein–Gordon equation for a particle of mass $|\mu|\hbar/c$:

$$\begin{aligned}&(-\partial_0^2 + \partial_1^2 + \partial_2^2 + \partial_3^2)\psi \\ &\quad = D^2\psi = D(\mu\psi) = \bar{\mu}D\psi = |\mu|^2\psi.\end{aligned}$$

It is noteworthy that one can obtain the equations only of massive and massless particles but not of imaginary mass tachyons.

Our equation is certainly translation invariant, and we shall show later that it is also invariant under Lorentz tran-

formations, so that despite its strangeness it does represent a genuine relativistic wave equation.

To get more feel for its significance we rewrite it in terms of the Fourier transform

$$(\mathcal{F}\psi)(p) = \int_{\mathbf{R}^4} e^{i\eta(p,x)}\psi(x)dx,$$

where η denotes the Lorentz-invariant bilinear form used to define $C^{1,3}$. One easily checks that the transform of the conjugate of ψ is

$$(\mathcal{F}\kappa\psi)(p) = (\mathcal{F}\psi)(-p),$$

so that the antilinear Dirac equation transforms to

$$\gamma(p)(\mathcal{F}\psi)(-p) = \mu(\mathcal{F}\psi)(p).$$

For massless particles, when $\mu = 0$ the antilinearity can be removed by conjugation and the equation reduces to the usual Weyl equation. Otherwise the corresponding Klein–Gordon equation ensures that $\mathcal{F}\psi$ is supported on the two-sheeted mass hyperboloid $\eta(p,p) = -|\mu|^2$, so that $\mathcal{F}\psi$ can be chosen arbitrarily on one sheet of the hyperboloid and the Dirac equation then determines its value on the other sheet. This shows that the equation does have nontrivial solutions, and indicates that its antilinearity is basically linked to the fact that time reversal is represented antilinearly.

We now return to the question of Lorentz invariance. To this end we must first describe the spin representation of the pseudo-orthogonal groups in this setting. We exploit the Freudenthal–Eckmann approach: The identity

$$\gamma(e_j)\gamma(v) = 2Q(e_j,v) - \gamma(v)\gamma(e_j)$$
$$= \gamma\left(2\frac{Q(e_j,v)}{Q(e_j,e_j)}e_j - v\right)\gamma(e_j),$$

still holds, and shows that $\gamma(e_j)$ implements the reflection in the hyperplane normal to e_j. Every element Λ of the proper pseudo-orthogonal group is the product of an even number of such reflections and so represented by a linear operator $\Gamma(\Lambda)$. By construction, this spin representation Γ satisfies

$$\Gamma(\Lambda)\gamma(v)\Gamma(\Lambda)^{-1} = \gamma(\Lambda v).$$

When $q+p$ is even, the hyperplane reflections have determinant -1 and so are not proper transformations. By adjoining them we can extend Γ to a corepresentation of the whole pseudo-orthogonal group. (When $q+p$ is odd the hyperplane reflections are proper transformations, so that there are both linear and antilinear transformations implementing these elements.)

If one follows the above constructions through for the Lorentz group then one obtains its usual projective representation as $\mathrm{SL}(2,\mathbf{C})$. We may then define a representation U of the Poincaré group on space-time wave functions by

$$(U(\Lambda,a)\psi)(x) = \Gamma(\Lambda)\psi(\Lambda^{-1}(x-a)),$$

where Λ is a Lorentz transformation and a a space-time translation. We can also Fourier transform U to act on momentum space wave functions:

$$(\mathcal{F}U(\Lambda,a)\psi)(p) = e^{i\eta(p,a)}\Gamma(\Lambda)(\mathcal{F}\psi)(\Lambda^{-1}p).$$

Since the antilinear Dirac equation is clearly translation-invariant we need only check its Lorentz invariance and this follows by direct calculation:

$$\gamma(p)(\mathcal{F}U(\Lambda)\psi)(-p)$$
$$= \gamma(p)\Gamma(\Lambda)(\mathcal{F}\psi)(-\Lambda^{-1}p)$$
$$= \Gamma(\Lambda)\gamma(\Lambda^{-1}p)(\mathcal{F}\psi)(-\Lambda^{-1}p)$$
$$= \Gamma(\Lambda)\mu(\mathcal{F}\psi)(\Lambda^{-1}p) = \mu(\mathcal{F}U(\Lambda)\psi)(p).$$

In fact, we may obtain a much more precise description of the behavior of the solutions of our equation under the action of the Poincaré group.

Theorem 2: The representation U of the Poincaré group on solutions of the antilinear Dirac equation is equivalent to the irreducible representation with mass $|\mu|\hbar/c$ and spin $\frac{1}{2}$.

Proof: For each p in the positive mass hyperboloid ($p_0 > 0$) we choose a Lorentz transformation $\Lambda(p)$ such that $\Lambda(p)\cdot e_0 = p$. For such p we now define the transformation T from the solution space of the antilinear Dirac equation to (complex-valued) functions on the positive mass hyperboloid by

$$(T\psi)(p) = \Gamma(\Lambda(p))^{-1}(\mathcal{F}\psi)(p).$$

It is easy to calculate that

$$(TU(\Lambda,a)\psi)(p) = e^{i\eta(p,a)}\Gamma(\Lambda(p)^{-1}\Lambda\Lambda(\Lambda^{-1}p))$$
$$\times(T\psi)(\Lambda^{-1}p).$$

The right-hand side is the standard Wigner form of the irreducible representation,[5] Sec. 6 C.

Conversely, given a function ϕ on the positive mass hyperboloid we can define a solution of the antilinear Dirac equation by setting

$$(T^{-1}\phi)(p)$$
$$= \begin{cases} \Gamma(\Lambda(p))\phi(p), & \text{when } p_0 > 0, \\ \mu^{-1}D\Gamma(\Lambda(p))\phi(-p), & \text{when } p_0 < 0. \end{cases}$$

Remark: It should be noted that despite our earlier comments about the solutions of the Dirac equation forming only a linear space, we have now proved the equivalence to a complex representation. The resolution of this paradox lies in the fact that the transformation T and its inverse are only real linear. We can, however, use them to carry back the complex structure on the irreducible representation space, setting $I = T^{-1}iT$. In fact, I is the standard complex structure of quantum field theory, which multiplies by $\pm i$ according to whether the energy is positive or negative. This means that the free-field theory can easily be constructed in the usual way. The standard Fock space theory will contain only electrons, but by going to other quasifree states such as the KMS state at a nonzero temperature, a theory which includes positrons can be constructed. They arise in much the same way that holes appear in solid-state theory. The complex structure I commutes with the Dirac operator, but not with the position operators, which makes the interactions of the antilinear Dirac electrons with other fields rather subtle. They will be discussed in a separate paper.[6]

IV. THE SUPER-POINCARÉ ALGEBRA

The Clifford algebras form a prototype for the more general situation in which the even part of a superalgebra g_0 is central.

Theorem 3: Let ρ be an irreducible corepresentation of

the superalgebra g whose even subalgebra g_0 is central, and define the bilinear form $Q_\rho(u,v) = \frac{1}{2}\rho([u,v])$ on g_1. Then the restriction of ρ to g_1 factorizes through the Clifford algebra defined by Q_ρ.

Proof: By Lemma 1 we know that ρ maps g_0 to multiples of the identity, so that Q_ρ is a real valued bilinear form, which is, moreover, clearly symmetric. We also have for all u and v in g_1

$$[\rho(u),\rho(v)]_+ = \rho([u,v]) = 2Q_\rho(u,v),$$

from which the assertion of the theorem follows immediately.

Remark: Of course, the form Q_ρ is usually degenerate, and elements in the radical must map to 0, since they are self-adjoint and satisfy

$$\rho(u)^2 = Q_\rho(u,u).$$

An important example of this occurs when g is the supertranslation subalgebra of the super-Poincaré algebra.[7] In this case $g_0 \cong \mathbf{R}^4$ is the Abelian Lie algebra of the space-time translations, and g_1 consists of the (real) Majorana spinors. More precisely, if we let η denote the Lorentz invariant bilinear form

$$\eta(x,y) = -x_0y_0 + x_1y_1 + x_2y_2 + x_3y_3,$$

then the corresponding Clifford algebra $C^{1,3}$ has a four-dimensional real representation on the space of Majorana spinors. The space of spinors has a Lorentz-invariant symplectic form c with respect to which the generators of the Clifford algebra act skew adjointly. [In conventional notation $c(u,v) = -u^t\gamma_0 v$.] We then define the superbracket $[u,v]$ of two elements u and v in g_1 to be the unique element of g_0 satisfying

$$\eta([u,v],y) = c(u,\gamma(y)v),$$

for all $y \in g_0$. As already hinted, g_0 is taken to be central in g.

We already know that the restriction to g_0 of an irreducible corepresentation must just be a real-valued linear functional on g_0. It must, therefore, have the form

$$\rho_p(x) = \eta(x,p),$$

for some $p \in g_0$. We are, therefore, led to the problem of finding the corepresentations of the Clifford algebra defined by the form

$$\rho_p([u,v]) = \eta([u,v],p) = c(u,\gamma(p)v).$$

This form has rank 4 when p is timelike and rank 2 when p is lightlike (null). In both cases it is positive semidefinite. Since, as we have seen in the preceding section, the Clifford algebra $C^{0,2}$ has a one-dimensional irreducible corepresentation it is possible to find a one-dimensional light-like corepresentation of the supertranslation algebra. At first sight this promises to reduce the size of the multiplets needed in a relativistic supersymmetric theory, but unfortunately this advantage is lost as soon as one builds in the effect of the Lorentz transformations.

The Lorentz group $L = \mathrm{SL}(2,C)$ acts on both the even and odd parts of g, and since both η and c are Lorentz-invariant it preserves the superbracket. We may, therefore, form the semidirect product of the Lorentz Lie algebra with g to obtain the super-Poincaré algebra. The obvious strategy for constructing corepresentations is to induce them by combining the method for inducing corepresentations of groups described in Ref. 2 with some form of superalgebra inducing such as that given in Ref. 7.

The little group L_0 that stabilizes the lightlike vector $p = (1,0,0,1)$ is the upper triangular subgroup of matrices of the form

$$\begin{pmatrix} e^{i\theta} & z \\ 0 & e^{-i\theta} \end{pmatrix},$$

for $\theta \in \mathbf{R}$ and $z \in \mathbf{C}$. The action of this element on the two-dimensional space whose Clifford algebra appears is by rotation through θ. Recalling the discussion of the spin representation in Sec. III we easily see that this is implemented on the one-dimensional corepresentation of $C^{0,2}$ by multiplication by $\exp(i\theta/2)$, for

$$e^{i\theta/2}(u_1 + iu_2)\kappa e^{-i\theta/2} = e^{i\theta/2}(u_1 + iu_2)e^{i\theta/2}\kappa = e^{i\theta}(u_1 + iu_2)\kappa.$$

Now, $\theta \to \exp(i\theta/2)$ is a projective representation of L_0, whose multiplier σ is ± 1 valued. In order to carry out the induction we need to extend σ to a multiplier on the whole of $\mathrm{SL}(2,\mathbf{C})$. Moreover, to be compatible with the antilinear structure we require it to be real valued. Since σ must also be unitary, this forces it to be ± 1 valued. On the other hand we know that all multipliers are trivial on $\mathrm{SL}(2,C)$, so that for some function λ we have

$$\sigma(x,y) = \lambda(x)\lambda(y)/\lambda(xy),$$

for all $x,y \in \mathrm{SL}(2,\mathbf{C})$. Since σ takes only the values ± 1 we may square this identity to get

$$\lambda(xy)^2 = \lambda(x)^2\lambda(y)^2,$$

showing that λ^2 is a character. Since the only one-dimensional representation of $\mathrm{SL}(2,\mathbf{C})$ is trivial, this means that λ is ± 1 valued. This, however, is inconsistent with the known behavior on the little group, where $\exp(i\theta/2)$ also trivializes σ. This means that λ can differ from $\exp(i\theta/2)$ on L_0 only by a character and it is easy to see that no such characters exist.

To avoid this problem one must start with a larger corepresentation of the supertranslations, but this forfeits the advantage of being able to reduce the size of the supersymmetric multiplets.

Of course, the arguments that we have used are peculiar to the super-Poincaré group, and do not necessarily hold in other cases. For example, the Euclidean group in two dimensions has a supersymmetric extension similar to the super-Poincaré group. In this case the little groups of nontrivial irreducible corepresentations of the supertranslation subalgebra are trivial, so that there are no obstacles to the inducing procedure.

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The electroweak interaction as a relativistic symmetry

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The electroweak gauge group arises naturally in a theory that uses an antilinear instead of a linear Dirac operator.

I. INTRODUCTION

In this paper we shall show that the standard Weinberg–Salam theory of the electroweak interactions,[1-3] fits naturally into a framework in which one starts with a Dirac operator which is antilinear rather than linear. In particular, the SU(2) gauge group appears quite naturally, as a group of intertwining operators.

Antilinear Dirac operators were considered in Ref. 4, to which this paper is a sequel. There it was shown that the Clifford algebra $C^{1,3}$ of the space $\mathbf{R}^4$ with the Minkowski inner product

$$\eta(x,y) = -x_0y_0 + x_1y_1 + x_2y_2 + x_3y_3$$

has a corepresentation on a two-dimensional space V_2, with the generators represented by the antilinear operators

$$\gamma_a v_a = \gamma(v) = \begin{pmatrix} v_2 + iv_1 & i(v_0 - v_3) \\ -i(v_0 + v_3) & v_2 - iv_1 \end{pmatrix}\kappa,$$

where κ is complex conjugation. In terms of the usual Pauli matrices and

$$\sigma_{\pm}(v) = (v_0 \pm v_1\sigma_1 \pm v_2\sigma_2 \pm v_3\sigma_3),$$

we may write

$$\gamma(v) = -\sigma_-(v)\sigma_2\kappa.$$

With the aid of these antilinear operators it was possible to construct a two-component massive Dirac equation:

$$D\psi = \mu\psi,$$

where $D = \gamma(\partial_0,\partial_1,\partial_2,\partial_3)$. For nonzero μ this equation was found to pick out a single irreducible representation of the Poincaré group with spin $\frac{1}{2}$ and mass $|\mu|\hbar/c$, while for zero μ one recovers the Weyl equation. Two features of this analysis suggest that it might well provide a convenient context for discussion of the electroweak forces: First, the electron and neutrino are described by wave functions with the same number of components, and, second, the resulting particle mass depends only on $|\mu|$, so that the theory carries a physically redundant phase strongly suggestive of a gauge symmetry.

Any change in the phase of μ will cause a compensating phase change in ψ. For definiteness suppose that ψ is multiplied by $\exp(iG)$. Then the antilinearity of the Dirac operator means that

$$De^{iG}\psi = e^{-iG}D\psi = e^{-iG}\mu\psi = e^{-2iG}\mu(e^{iG}\psi).$$

In other words μ has changed by a factor of $\exp(-2iG)$. To obtain a gauge theory we allow G (and, therefore, also μ) to be a function on space-time, and introduce a $U(1)$ valued connection ∇. We now adjust the notation and write D for the operator $\gamma(\nabla)$. In the equation

$$D\psi = \mu\psi,$$

μ now represents a field, which, from its gauge dependence, has a $U(1)$ charge -2 times that of ψ.

We shall not pursue this approach further because it turns out that with a small modification it can be made to include the weak force as well. This will be explained in the next section. We shall then classify the Lorentz invariant forms and show that these are just the usual currents and interaction terms, enabling us to reconstruct the Lagrangian density of the standard model.

We shall follow the physicists' convention of denoting complex conjugation by an asterisk and Hermitian conjugates or adjoints by a dagger. The superscript τ will denote a transpose.

II. THE ELECTROWEAK GAUGE GROUP

In practice it is now more usual to take

$$-\eta(x,y) = x_0y_0 - x_1y_1 - x_2y_2 - x_3y_3,$$

as the Lorentz invariant form on Minkowski space rather than η. The effect of this on the corepresentation theory is quite remarkable. According to the criterion established in Ref. 4, Corollary B to Theorem 1 the irreducible corepresentations of the Clifford algebra $C^{3,1}$ have the same dimension as the irreducible representations, that is 4. Indeed, one may take the block form

$$\tilde{\gamma}(v) = \begin{pmatrix} 0 & \gamma(v) \\ -\gamma(v) & 0 \end{pmatrix},$$

as a typical generator, with v in $\mathbf{R}^4$. In similar block form the Lorentz transformation Λ may be represented by

$$\tilde{\Gamma}(\Lambda) = \begin{pmatrix} \Gamma(\Lambda) & 0 \\ 0 & \Gamma(\Lambda) \end{pmatrix},$$

where Γ denotes the natural representation of the Lorentz transformations as elements of $SL(2,C)$, (cf. Ref. 4, Sec. III).

For many purposes it is more convenient to consider the four-dimensional corepresentation space as the tensor product of 2 two-dimensional spaces:

$$V_4 = \mathscr{H} \otimes V_2.$$

The space V_2 is the corepresentation space for the Clifford algebra of η used in the first section. Introducing the matrix $\tau = -i\sigma_2$ we than have $\tilde{\gamma}(v) = \tau\kappa \otimes \gamma(v)$. The Lorentz action takes the form

$$\tilde{\Gamma}(\Lambda) = 1 \otimes \Gamma(\Lambda),$$

By way of compensation for having to double the dimension there are now more intertwining operators. In fact,

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since these necessarily commute with the Lorentz transformations they must take the form $\Phi \otimes 1$. The intertwining property then means that $\tau\Phi^*\tau = \Phi$ which means that

$$\Phi = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

for suitable complex numbers a and b. The algebra of such operators is isomorphic to the quaternions. Moreover, the unit quaternions, which are those satisfying $|a|^2 + |b|^2 = 1$, form the group SU(2). Indeed the corresponding intertwining matrices give the direct sum of two copies of the natural representation of SU(2).

It is not easy to construct a Dirac operator,

$$\tilde{D} = \tilde{\gamma}(\nabla) = \begin{pmatrix} 0 & \gamma(\nabla) \\ -\gamma(\nabla) & 0 \end{pmatrix}$$

$$= \tau\kappa \otimes D.$$

However, if we simply replace D by $\tilde{D}$ in the Dirac equation then the reversed sign of η leads to imaginary mass tachyon solutions. Fortunately, the intertwining operators provide a way out, for we can choose any intertwining operator I whose square is -1 and then take as the new Dirac operator $I\tilde{D}$. One particularly convenient choice is to take $I = -\tau \otimes 1$ since then we have $\tilde{D} = \kappa \otimes D$. The corresponding Dirac equation

$$\tilde{D}\Psi = \mu\Psi,$$

in which Ψ is now a four-component spinor, clearly breaks into the direct sum of two of the previous two component equations.

The new feature that emerges, however, is that we are free to multiply the operator I by any unit quaternion. This provides a natural setting for the appearance of SU(2) as a gauge group for the theory, and means that we must also regard ∇ as a $U(1)\times SU(2)$ connection. To conform with standard conventions we define compatible actions of an element $u \in U(1)$ by letting it multiply by u on V_4 and $\mathscr{H}$, and by u^{-2} on V_2. We shall henceforth assume that the appropriate connections are used in the definitions of D and $\tilde{D}$. (The relationship $\tilde{D} = \kappa \otimes D$ will then fail since D and $\tilde{D}$ will involve different connections.)

III. INVARIANT FORMS

In order to obtain Lagrangian density functions we need to construct gauge and Lorentz invariant functions of the wave functions. We start by considering the case of the two-dimensional spinors ψ.

Since the Lorentz group SL(2,C) does not act unitarily on spinors it is easy to see that there are no invariant sesquilinear forms, that is expressions of the form $\psi^* G\psi$. On the other hand there is an invariant skew symmetric bilinear form derived from the exterior product on $V_2 \simeq \mathbf{C}^2$:

$$\epsilon(\phi,\psi) = \phi_1\psi_2 - \phi_2\psi_1,$$

and, up to multiples, ϵ is the only invariant bilinear form. It is easy to check that for any vector v in $\mathbf{R}^4$ we have

$$\epsilon(\phi,\gamma(v)\psi) + \epsilon(\psi,\gamma(v)\phi))^* = 0.$$

This means that $\epsilon(\psi,\gamma(v)\psi)$ is imaginary. In terms of $\tau = -i\sigma_2$ we may write

$$\epsilon(\phi,\gamma) = \phi^{\mathrm{T}}\tau\psi$$

and

$$\epsilon(\phi,\gamma(v)\psi) = -\phi^{\mathrm{T}}\tau\sigma_-(v)\sigma_2\kappa\psi$$
$$= i\phi^{\mathrm{T}}\sigma_+(v)^{\mathrm{T}}\psi^*$$
$$= i\psi^\dagger\sigma_+(v)\phi.$$

On substituting ∇ for v and using Leibniz' rule we similarly obtain

$$\epsilon(\psi,D\psi) = -i\psi^\dagger\sigma_+(\nabla)\psi + i\partial_\alpha(\psi^\dagger\sigma_\alpha\psi).$$

Apart from the unimportant divergence term this is just the formula for the right-handed part of the standard Dirac current.

Our next task is to identify the invariant forms on V_4. It is clear from the preceding analysis in V_2 that there are no Lorentzian invariant sesquilinear forms, and that any invariant bilinear form can be written as $B \otimes \epsilon$, where B is a bilinear form on $\mathscr{H}$. The only SU(2)-invariant form on $\mathscr{H}$ is again ϵ so that adding the requirement of SU(2) gauge invariance reduces the possibilities to just scalar multiples of $s = \epsilon \otimes \epsilon$. Since each ϵ is skew symmetric the bilinear form s is symmetric. Moreover, since τ is easily seen to be symmetric with respect to ϵ it follows that $\tilde{\gamma}(v)$ is conjugate skew symmetric with respect to s for any space-time vector v, that is

$$s(\Phi,\tilde{\gamma}(v)\Psi) + s(\Psi,\tilde{\gamma}(v)\Phi)^* = 0.$$

Following the same procedure as in two dimensions we have

$$s(\Phi,\Psi) = \Phi^{\mathrm{T}}(\tau \otimes \tau)\Psi,$$

and

$$s(\Phi,\tilde{\gamma}(v)\Psi) = \Phi^{\mathrm{T}}(\tau \otimes \tau)(\tau\kappa \otimes \sigma_-(v)\sigma_2\kappa)\Psi$$
$$= i\Phi^{\mathrm{T}}(1 \otimes \sigma_2\sigma_-(v)\sigma_2)\Psi^*.$$

In terms of the charge conjugates

$$\Psi_c = (\sigma_3 \otimes \tau)\Psi^*,$$

and Φ_c, this may be written as

$$s(\Phi,\tilde{\gamma}(v)\Psi) = i\Phi_c^\dagger(1 \otimes \sigma_-(v))\Psi_c.$$

Replacing v by ∇ we obtain

$$s(\Psi,\tilde{D}\Psi) = i\Psi_c^\dagger(1 \otimes \sigma_-(\nabla))\Psi_c.$$

Regarded as a function of $l = \Psi_c$ this is the formula for the lepton current of a left-handed SU(2) doublet.

IV. THE ELECTROWEAK UNIFICATION

The full theory will contain fields of both kinds: ψ in V_2 and Ψ in V_4. These are linked by means of a Lorentz invariant imbedding of V_2 into V_4. We have already seen that such imbeddings exist and indeed, since $V_4 = \mathscr{H} \otimes V_2$, they are obtained by taking the tensor product with elements of $\mathscr{H}$. We therefore introduce the $\mathscr{H}$-valued field ϕ.

The natural coupling between such fields is given by

$$
\begin{aligned}
s(\phi\otimes\psi,\Psi) &= (\phi^{\tau}\otimes\psi^{\tau})(\tau\otimes\tau)\Psi \\
&= (\phi^{\tau}\otimes\psi^{\tau})(\tau\otimes\tau)(\sigma_3\otimes\tau)\Psi_c^{*} \\
&= -\Psi_c^{\dagger}(\sigma_3\otimes\tau)(\tau\otimes\tau)(\phi\otimes\psi) \\
&= -\Psi_c^{\dagger}(\sigma_1\otimes 1)(\phi\otimes\psi).
\end{aligned}
$$

The helicity representation of the ordinary Dirac matrix "γ_0" is $\sigma_1\otimes 1$, so that this is the standard interaction term.

Pulling the pieces together we see that the leptonic and Higgs part of the standard model Lagrangian may be expressed as

$$
\begin{aligned}
\mathscr{L} &= s(\Psi,\tilde{D}\Psi) - \epsilon(\psi,D\psi) + (m_e/\beta) \\
&\quad\times(s(\Psi,\phi\otimes\psi) + s(\Psi,\phi\otimes\psi)^{*}) \\
&\quad + \eta(\nabla\phi^{*},\nabla\phi) - \lambda(\phi^{*}\phi-\beta^2)^2,
\end{aligned}
$$

where β and λ are positive constants. The standard gauge curvature and 't Hooft terms may be added to this and the symmetry broken in the usual way to recover the standard model.

V. CONCLUDING REMARKS

At the expense of moving to a higher dimension it is always possible to linearize an antilinear mapping. If we define $V_8 = V_4\oplus V_4^{*}$, where V_4^{*} denotes the complex conjugate space, then the Clifford elements act linearly by mapping V_4 to V_4^{*} and vice versa. This linear representation of the Clifford algebra breaks up as the direct sum of two copies of the standard irreducible W, so that one may write $V_8 = \mathscr{H}\otimes W$. The SU(2) action is on $\mathscr{H}$ mixing the two copies of W, so that in the standard linear theory of the Dirac equation where one works on just one of the irreducible summands it is not directly visible. However, just as the action of the Clifford algebra on V_8 is the linearization of a nonlinear action on V_4, so that SU(2) action is the linearization of a nonlinear action on W. It is, in fact, well known that the irreducible linear representation of the Clifford algebra of $-\eta$ is "quaternionic." However, the action of the quaternions on the representation space is only real linear and not complex linear.

The space V_8 is large enough to encompass both the standard linear Dirac theory and this new variant. The neutrino and both helicity states of the electron find a place in it. It also inherits from the linear Clifford irreducibles an action of the full conformal group, SU(2,2) rather than just the Lorentz group. This suggests that it might be preferable to work with a theory at this level and break the conformal and weak gauge symmetry at the same time. We hope to return to this in a future paper.

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Superposition formulas for nonlinear superequations

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Nonlinear superequations, for which the general solution can be expressed algebraically in terms of a finite number of particular solutions, are obtained. They are based on the orthosymplectic supergroup OSP(m,$2n$) and its action on a homogeneous superspace. Superposition formulas are discussed for the cases $m = 1$, n arbitrary, and $m = 2$, $n = 1$. For OSP(2,2) the number of particular solutions needed to reconstruct the general solution depends on the dimension of the underlying Grassmann algebra, whereas for OSP(1,2n) it does not.

I. INTRODUCTION

A system of ordinary differential equations (ODEs) is said to allow a superposition formula, if its general solution $\mathbf{y}(t)$ can be expressed as a function of a finite number of particular solutions $\mathbf{y}_1,...,\mathbf{y}_m$ and a sufficient number of arbitrary constants $c_1,...,c_n$:

$$\mathbf{y}(t) = \mathbf{F}(\mathbf{y}_1(t),...,\mathbf{y}_m(t),c_1,...,c_n). \tag{1.1}$$

Lie[1] has shown that the necessary and sufficient condition for such a superposition formula to exist is that the ODEs have the form

$$\dot{\mathbf{y}}(t) = \sum_{k=1}^{r} Z_k(t)\xi_k(\mathbf{y}), \tag{1.2}$$

where the vector functions $\xi_k(\mathbf{y})$ are restricted by the condition that the differential operators,

$$X_k = \sum_{\mu=1}^{n} \xi_k^{\mu}(\mathbf{y})\frac{\partial}{\partial y^{\mu}}, \tag{1.3}$$

should generate a finite-dimensional Lie algebra L.

It has been shown[2] that a system of such equations can be associated with every homogeneous space $M \sim G/G_0$, where G is any finite-dimensional Lie group and G_0 is any closed continuous subgroup of G. The Lie algebra (1.3) of Lie's theorem is the algebra associated with G and $L_0 \subset L$, associated with G_0, is the algebra of vector fields vanishing at some point (the origin) of M. Special attention was devoted to indecomposable systems of equations, from which no proper subsystem can be split off, having a superposition formula of its own. Indecomposable systems of equations were shown to correspond to transitive primitive actions of G on M. The indecomposable systems of ODEs with superposition formulas were classified,[2] making use of the known classification of transitive primitive Lie algebras.[3-6]

A systematic study of indecomposable systems of ODEs with superposition formulas was undertaken in a series of recent articles.[7-12] We refer to the original articles for all details and implications. Such important equations as the matrix Riccati equation belong to this category.

As a direct motivation for the study of nonlinear superposition formulas let us just mention that these formulas, when they exist, are of great help in solving the equations and in establishing the properties of their sets of solutions. Moreover, equations with superposition formulas also have the Painlevé property (their solutions have no movable singularities, other than poles). In this context, group theory can be directly used to determine, whether a system of ODEs is integrable, or not. In a broader context, nonlinear ODEs with superposition formulas are related to completely integrable dynamical systems, where they occur as Bäcklund transformations.[13,14]

The concept of nonlinear ODEs with superposition formulas has recently been extended to nonlinear "superequations,"[15] involving even and odd Grassmann variables[16] as dependent variables and the ordinary variable t as the independent variable. The so-called "super-Riccati equations"[15] belong to such a category. The theory of such equations is based on Lie superalgebras,[17] the superposition formulas being obtained from the action of the corresponding Lie supergroups on homogeneous supermanifolds.[18]

Such superequations and their solutions are of interest for two complementary reasons. The first is that such equations occur in supersymmetrical physical theories, developed in a variety of different areas of physics.[19-22] Tools to solve superequations are hence needed and superposition formulas, if nothing else, reduce the problem of finding all solutions, to that of finding a finite number of particular ones. The second reason is that superequations can be used to represent in a compact form large (actually arbitrarily large) systems of ordinary equations. Indeed, once the dimension N of the underlying Grassmann algebra is specified and a basis $\Theta_1,\Theta_2,...,\Theta_N$ is chosen, each even or odd Grassmann variable can be expanded in terms of products of Θ_i.

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The superequations then reduce to usual ODEs for the expansion coefficients. The superposition formula for the superequation goes over into one for the usual ODEs. It will coincide with a formula that could be obtained directly from the action of some ordinary Lie group on an ordinary manifold. The "super" version will in general be much more compact. This approach is similar to the one advocated by Fatyga *et al.*,[23] who combined systems of nonlinear partial differential equations originating in fluid dynamics, into one Grassmann valued partial differential equation.

Our previous article[15] on superequations was restricted to considerations based on the orthosymplectic Lie supergroup OSP(1,2). In the present article, we first derive nonlinear superequations related to the action of the supergroup OSP(m,2n) on a homogeneous superspace for m and n arbitrary (Sec. II). In Sec. III, we obtain the superposition formulas for OSP(1,2n), with n arbitrary. For $n=1$, we need three particular solutions to form a fundamental set as is already known[15] but for $n\geqslant 2$ we need four, these results being independent of the dimension of the underlying Grassmann algebra. In Sec. IV we analyze the superposition formula for the special case of OSP(2,2). In this case it turns out that the number of particular solutions needed to obtain a superposition formula does depend on N, where N is the number of generators of the Grassmann algebra. We conclude in Sec. V.

II. SUPEREQUATIONS BASED ON THE OSP(m,2n) SUPERGROUP

In this section we first sum up some basic results on the Lie supergroup OSP(m,2n) and its superalgebra osp(m,2n). We then derive the nonlinear superequations related to the action of OSP(m,2n) on a homogeneous superspace. Finally, we show that these equations allow a superposition formula.

A. The supergroup OSP(m,2n) and its action on the superspace

Let us work with Θ_a, $a=1,\ldots,N$, a set of generators of a Grassmann algebra Λ_N.[16,18] They satisfy $\Theta_a\Theta_b+\Theta_b\Theta_a=0$, $a,b=1,\ldots,N$. The elements $1, \Theta_a, \Theta_a\Theta_b,\ldots$, where the indices in each product are all different, form a (2^N dimensional) basis of Λ_N. The elements of Λ_N will be called supernumbers and admit a decomposition into even and odd parts. They can be written, respectively,

$$x=a_0+\sum_{r=1}^{[N/2]} a_{i_1\cdots i_{2r}}\Theta_{i_1}\cdots\Theta_{i_{2r}}, \tag{2.1}$$

$$\Theta=\sum_{r=0}^{[(N-1)/2]} b_{i_1\cdots i_{2r+1}}\Theta_{i_1}\cdots\Theta_{i_{2r+1}}, \tag{2.2}$$

$$i_k\in\{1,\ldots,N\}, i_1<i_2<\cdots<i_{2r+1},$$

where a_0, $a_{i_1\cdots i_{2r}}$, $b_{i_1\cdots i_{2r+1}}\in F=\mathbb{R}$ or $\mathbb{C}$ and a_0 is called the body of the supernumber. We shall denote throughout the even (odd) supernumbers by Latin (Greek) letters. Note that the product of two odd supernumbers gives an even supernumber while the product of an even with an odd supernumber gives an odd supernumber. An even supernumber has a multiplicative inverse if its body is not zero. Since the odd supernumbers and the even supernumbers, which are products of odd ones have no body, they are not invertible.

We describe now the well-known properties[17] of the simple superalgebra osp(m,2n) and of the corresponding supergroup OSP(m,2n). They can be realized as the set of $(m+2n)\times(m+2n)$ matrices that satisfy, respectively,

$$M^{\mathrm{ST}}H+HM=0, \quad \mathcal{G}^{\mathrm{ST}}H\mathcal{G}=H,$$

$$H=\begin{pmatrix} I_m & 0 & 0\\ 0 & 0 & I_n\\ 0 & -I_n & 0\end{pmatrix} \tag{2.3}$$

where the superscript ST denotes the "supertransposition."[17] Explicitly, we have

$$M=\begin{pmatrix} M_1 & \mu_1 & \mu_2\\ \mu_2^T & C & A\\ -\mu_1^T & -D & -C^T\end{pmatrix},$$
$$M_1{}^T=-M_1, \quad A^T=A, \quad D^T=D \tag{2.4}$$

and

$$\mathcal{G}=\begin{pmatrix} G & \Gamma_1 & \Gamma_2\\ \Lambda_1^T & G_{11} & G_{12}\\ \Lambda_2^T & G_{21} & G_{22}\end{pmatrix}, \tag{2.5a}$$

where

$$\begin{aligned} &G^TG-\Lambda_1\Lambda_2^T+\Lambda_2\Lambda_1^T=I_m,\\ &\Gamma_1^T\Gamma_1+G_{11}^TG_{21}-G_{21}^TG_{11}=0,\\ &\Gamma_2^T\Gamma_2+G_{12}^TG_{22}-G_{22}^TG_{12}=0,\\ &\Gamma_1^T\Gamma_2+G_{11}^TG_{22}-G_{21}^TG_{12}=I_n,\\ &G^T\Gamma_1-\Lambda_1G_{21}+\Lambda_2G_{11}=0,\\ &G^T\Gamma_2-\Lambda_1G_{22}+\Lambda_2G_{12}=0. \end{aligned} \tag{2.5b}$$

In Eqs. (2.4) and (2.5) the elements of M_1, G, A, C, D, G_{ij} ($i,j=1,2$) are even supernumbers while the elements of μ_1, μ_2, Γ_1, Γ_2, Λ_1, Λ_2 are odd supernumbers. Also, M_1 and G are $m\times m$ matrices, A, C, D, G_{ij} are $n\times n$ matrices and finally $\mu_1,\mu_2,\Gamma_1,\Gamma_2,\Lambda_1,\Lambda_2$ are $m\times n$ matrices. The dimension d of OSP(m,2n) is given by

$$d\equiv(d_{\mathcal{G}},d_{\mathcal{C}})=\left(\frac{m(m-1)}{2}+2n^2+n,2mn\right),$$

where $d_{\mathcal{G}}$ ($d_{\mathcal{C}}$) is the number of even (odd) independent entries.

The supergroup OSP(m,2n) acts linearly on the superspace[18] formed, in particular, by supervectors of the type $X^T=(\xi^T\ X_1^T\ X_2^T)^T$. The even part $X_{\mathcal{G}}$ contains a $2n$-dimensional even vector $(X_1^T\ X_2^T)^T$ while the odd part $X_{\mathcal{C}}$ contains an m-dimensional odd vector ξ. The supernorm of X coincides in this case with the norm, i.e., we have

$$X^{\mathrm{ST}}HX\equiv X^THX=\xi^T\xi+X_1^TX_2-X_2^TX_1. \tag{2.6}$$

B. The nonlinear superequations

The nonlinear ODEs based on a Lie supergroup can be constructed using the usual procedure for Lie groups.[2] Indeed, let us first consider a maximal subsupergroup G^0 of OSP$(m,2n)$ leaving, for example, the n-dimensional supervector space of the type $(0\ 0\ y^T)^T$ invariant. We are then concerned with supervectors with supernorm equal to zero, as follows directly from (2.6). This subsupergroup G^0 is of dimension

$$d^0=\left(\frac{m(m-1)}{2}+n^2+\frac{n(n+1)}{2},nm\right)$$

and is described by matrices of the form

$$\mathcal{G}_0=\begin{pmatrix} G & \Gamma_1 & 0 \\ 0 & G_{11} & 0 \\ -G_{11}^{-T}\Gamma_1^T G & G_{21} & G_{11}^{-T} \end{pmatrix}, \tag{2.7}$$

with

$$G^TG=I_m,\quad G_{11}^TG_{21}-G_{21}^TG_{11}+\Gamma_1^T\Gamma_1=0. \tag{2.8}$$

Secondly, we need to construct a realization of the homogeneous superspace $M\equiv\text{OSP}(m,2n)/G^0$ of dimension

$$d-d^0=(n(n+1)/2,nm).$$

We will use both homogeneous and affine coordinates on M which are, respectively,

$$U=\begin{pmatrix}\xi\\ X\\ Y\end{pmatrix}\quad\text{and}\quad W=\begin{pmatrix}\eta\\ Z\end{pmatrix}=\begin{pmatrix}\xi Y^{-1}\\ XY^{-1}\end{pmatrix},\quad \det Y\neq 0. \tag{2.9}$$

The homogeneous coordinates U are formed by an $(m\times n)$-odd supervector ξ and two $(n\times n)$-even matrices X and Y. They satisfy the isotropy condition

$$U^{\text{ST}}HU=\xi^T\xi+X^TY-Y^TX=0. \tag{2.10}$$

There is a redundancy in such coordinates since U and UK, where K is an $(n\times n)$-even nonsingular matrix, represent the same point. In order to avoid this redundancy we introduce the affine coordinates W (in the neighborhood of the origin we have $\det Y\neq 0$). The isotropy condition (2.10) thus becomes

$$Z^A\equiv\tfrac{1}{2}(Z-Z^T)=\tfrac{1}{2}\eta^T\eta, \tag{2.11}$$

so that the antisymmetric part of the matrix Z is not independent. The coordinates on M are then identified with the components of the two matrices $Z^S\equiv\frac{1}{2}(Z+Z^T)$ and η.

Finally we can write the nonlinear ODEs corresponding to the action of OSP$(m,2n)$ on M. In homogeneous coordinates we have a set of linear equations

$$\dot U=MU,\quad \dot U=\frac{dU}{dt}, \tag{2.12}$$

with the nonlinear constraint (2.10) and the redundancy $U\cong UK$. In affine coordinates, we eliminate the redundancy and use the constraint (2.11) to find the nonlinear superequations. These are given by

$$\dot\eta=\mu_2+\mu_1Z^S+\eta(DZ^S+C^T)+(M_1+\eta\mu_1^T+\tfrac{1}{2}\mu_1\eta^T+\tfrac{1}{2}\eta D\eta^T)\eta, \tag{2.13a}$$

$$\dot Z^S=A+\tfrac{1}{2}(\mu_2^T\eta-\eta^T\mu_2)+\tfrac{1}{4}\eta^T(\eta\mu_1^T+\mu_1\eta^T+\eta D\eta^T)\eta+Z^S(C^T+\tfrac{1}{2}\mu_1^T\eta)+(C-\tfrac{1}{2}\eta^T\mu_1)Z^S+Z^SDZ^S. \tag{2.13b}$$

The nonlinearities of (2.13) are quadratic in Z^S but up to quartic in η. The quantities μ_i, M_1, A, C, D are given functions of t.

C. Existence of a superposition formula

The action of OSP$(m,2n)$ on the homogeneous space M is given in affine coordinates by

$$\eta(t)=(G\eta_0+\Gamma_1Z_0+\Gamma_2)(\Lambda_2^T\eta_0+G_{21}Z_0+G_{22})^{-1}, \tag{2.14a}$$

$$Z(t)=(\Lambda_1^T\eta_0+G_{11}Z_0+G_{12})\times(\Lambda_2^T\eta_0+G_{21}Z_0+G_{22})^{-1}. \tag{2.14b}$$

A superposition formula for Eqs. (2.13) will have the form (2.14), where $(\eta(t),Z(t))$ is a general solution and (η_0,Z_0) are arbitrary constant matrices related to the initial conditions [both are constrained by (2.11)]. The matrix functions $G(t)$, $G_{ij}(t)$, $\Gamma_i(t)$, $\Lambda_i(t)$ $(i,j=1,2)$ will be determined in terms of a fixed finite number m of particular solutions.

The reconstruction of $\mathcal{G}(t)$ follows the same procedure as in the case of Lie groups.[7-12] Indeed, we take the m particular solutions $U_k(t)$ $(k=1,...,m)$ in homogeneous coordinates (assumed to be known with the ambiguity inherent in the redundancy $U\sim UK$) and write

$$U_k(t)=\mathcal{G}(t)U_k(0),\quad \text{for } k=1,2,...,m. \tag{2.15}$$

We then solve this set of equations for the matrix elements of $\mathcal{G}(t)$. This set will determine $\mathcal{G}(t)$ uniquely if $\{U_1(t),...,U_m(t)\}$ is a fundamental set of solutions, i.e., if the joint stabilizer in OSP$(m,2n)$ of the m initial condition matrices $U_1(0),...,U_m(0)$ is just the identity transformation.

We have to be more precise about the meaning of an identity transformation in the case of a supergroup element acting on a supervector space. Indeed, since we act on supervectors of the form (2.9), the group element $\mathcal{G}(0)$ acting as the identity transformation on $U_k(0)$ has the form

$$\mathcal{G}(0)=\begin{pmatrix}I_m & 0\\ 0 & I_{2n}\end{pmatrix}+(1+(-1)^N)\begin{pmatrix}B & 0\\ 0 & 0\end{pmatrix}\left(\prod_{j=1}^{N}\Theta_j\right), \tag{2.16}$$

where B is an $(m\times m)$-antisymmetric matrix, i.e., $\mathcal{G}(0)$ is the identity if N is odd while there is an additional element if N is even that acts trivially on the entire superspace.

In the following sections, we restrict ourselves to the nonlinear superposition formulas corresponding to the specific cases of OSP$(1,2n)$ and OSP$(2,2)$.

III. SUPERPOSITION FORMULA FOR THE EQUATIONS BASED ON OSP(1,2n)

The supergroup OSP$(1,2n)$ is of dimension $d=(n(2n+1),2n)$ and the homogeneous space

$\mathrm{OSP}(1,2n)/G^0$ is then of dimension $(n(n+1)/2,n)$. In Eq. (2.13), η, μ_1, μ_2 are $(1\times n)$-odd supervectors and $M_1 = 0$. In the formula (2.14), Γ_1, Γ_2, Λ_1, and Λ_2 are also $(1\times n)$-odd supervectors while $G \equiv g$ is a (1×1)-even matrix, i.e., an even supernumber.

In order to show clearly how the procedure of reconstruction of the group element $\mathcal{G}(t) \in \mathrm{OSP}(1,2n)$ entering in the formula (2.14) works, it is useful to first consider the case $n = 1$ and then generalize to arbitrary n.

A. Reconstruction of the supergroup element for $n=1$

We proved in Ref. 15 that a fundamental set of *three* solutions is needed to be able to write the general solution of Eq. (2.13) in the OSP(1,2) context. The reconstruction was realized by specifying the number of generators of the Grassmann algebra under consideration. Here, we add a new result, namely a reconstruction that is independent of the number of generators of the Grassmann algebra and is performed in all generality.

1. Fundamental set of solutions

Let us recall the theorem that gives the number and the form of the independent solutions.

Theorem: A fundamental set of solutions of the "super-Riccati equations" (2.13) consists of three solutions $W_i = (\eta_i, z_i)\,(i = 1,2,3)$ with initial conditions satisfying

$$\eta_i(0)\eta_k(0) + z_k(0) - z_i(0) = (1-\delta_{ik})A_{ik}, \quad i,k = 1,2,3,$$
$$\eta_1(0)(z_2(0) - z_3(0)) + \eta_2(0)(z_3(0) - z_2(0)) + \eta_3(0)(z_1(0) - z_2(0)) = B\Theta, \tag{3.1}$$

where A_{ik} and B are arbitrary even invertible elements of the Grassmann algebra and Θ is an arbitrary odd element.

Note that this means in particular that, in homogeneous coordinates, three initial vectors $U_i(0)$ corresponding to W_i can be transformed into

$$U_1(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \quad U_2(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad U_3(0) = \begin{pmatrix} \Theta \\ x \\ y \end{pmatrix}, \tag{3.2}$$

where x and y are invertible. The proof of the theorem is given in Ref. 15 and it consists essentially in showing that the subsupergroup of OSP(1,2) leaving all three vectors (3.2) invariant is the identity group.

2. Reconstruction

The reconstruction procedure is almost the same as the one given in our previous article.[15] In fact it differs only in the last step and leads to the determination of all the group elements *independently* of the number of Grassmann generators.

Indeed, making use of the orthogonality conditions and the first two particular solutions, we see that only one entry remains unknown. This means that the knowledge of the even part of the third solution is sufficient to obtain the remaining unknown.

Explicitly, we proceed as follows. First, using the two solutions W_1 and W_2 we find [$\Gamma_i = \gamma_i$, $\Lambda_i = \lambda_i$ and $G_{ij} = g_{ij}$, $i,j = 1,2$ in (2.5a)]

$$\gamma_1 = z_2^{-1}\eta_2 g_{11}, \quad \gamma_2 = \eta_1 g_{22},$$
$$g_{12} = z_1 g_{22}, \quad g_{21} = z_2^{-1} g_{11}. \tag{3.3}$$

Among the orthogonality conditions (2.5b), we find four nontrivial equations, i.e.,

$$g^2 - 2\lambda_1\lambda_2 = 1, \tag{3.4a}$$
$$g_{11}g_{22} - g_{21}g_{12} + \gamma_1\gamma_2 = 1, \tag{3.4b}$$
$$g\gamma_1 - \lambda_1 g_{21} + \lambda_2 g_{11} = 0, \tag{3.4c}$$
$$g\gamma_2 - \lambda_1 g_{22} + \lambda_2 g_{12} = 0. \tag{3.4d}$$

The relations (3.4c) and (3.4d) together with (3.3) lead to the determination of λ_1 and λ_2 up to the factor g, i.e.,

$$\lambda_1 = g(z_1\eta_2 - z_2\eta_1)(z_1 - z_2)^{-1},$$
$$\lambda_2 = g(\eta_2 - \eta_1)(z_1 - z_2)^{-1}. \tag{3.5}$$

Equation (3.4a) gives

$$g = [(z_1 - z_2)(z_1 - z_2 + 2\eta_2\eta_1)^{-1}]^{1/2}. \tag{3.6}$$

The plus sign has been fixed in the square root using the fact that $g(0) = 1$ and $g(t)$ is a continuous function of t. Equation (3.4b) gives g_{22} in terms of g_{11}, i.e.,

$$g_{22} = z_2(z_2 - z_1 - \eta_1\eta_2)^{-1} g_{11}^{-1}. \tag{3.7}$$

At this stage, everything is known in terms of g_{11}. We use the third solution W_3 and in particular the equation

$$z_3 = (\lambda_1\Theta + g_{11}x + g_{12}y)(\lambda_2\Theta + g_{21}x + g_{22}y)^{-1} \tag{3.8}$$

to determine g_{11}. Equation (3.8) is a quadratic equation for g_{11} and the unicity of the solution is again assured by the continuity of g_{11} and the fact that $g_{11}(0) = 1$. We have, finally

$$g_{11} = \frac{(\lambda_1 - \lambda_2 z_3)\Theta}{2xz_2^{-1}(z_3 - z_2)} + \left[\frac{yz_2^2(z_3 - z_1)}{x(z_3 - z_2)(z_1 - z_2 + \eta_1\eta_2)}\right]^{1/2}, \tag{3.9}$$

where λ_1 and λ_2 are given by (3.5) with (3.6).

B. Reconstruction of the supergroup element for $n \geqslant 2$

We have the set (2.13) of n equations in the odd variables η and $n(n+1)/2$ equations in the even variables Z^S. We want to show that in this case *four* particular solutions are needed to write the general solution, independently of the number of Grassmann generators.

1. Fundamental set of solutions

We choose a convenient fundamental set of solutions by fixing the homogeneous coordinates of four initial conditions as

$$U_1(0) = \begin{pmatrix} 0 \\ 0 \\ I \end{pmatrix}, \quad U_2(0) = \begin{pmatrix} 0 \\ I \\ 0 \end{pmatrix},$$
$$U_3(0) = \begin{pmatrix} 0 \\ I \\ I \end{pmatrix}, \quad U_4(0) = \begin{pmatrix} \alpha \\ X \\ I \end{pmatrix}, \tag{3.10}$$

where $\alpha = (1,\ldots,1)\Theta$, $X = \mathrm{diag}\,(a_1,\ldots,a_n)$, $a_i \neq a_j$ for $i \neq j$, Θ

being a fixed odd Grassmann number and the a_i's ordinary numbers.

We proceed to show that the joint isotropy group of these four initial conditions is the identity group. Imposing $\mathcal{G}U_i(0) \cong U_i(0)$ for $i=1$ and 2 and using the orthosymplecticity conditions (2.5b) we find that the isotropy group G_{12} of the first two solutions is realized by block diagonal matrices

$$\mathcal{G}_0 = \mathrm{diag}(g, G_{11}, G_{11}^{-T}). \tag{3.11}$$

Requiring $\mathcal{G}_0\, U_3(0) \cong U_3(0)$ we obtain

$$G_{11} G_{11}^T = I, \tag{3.12}$$

i.e., $G \in O(n,F)$. Finally the stabilization of the vector $U_4(0)$ implies

$$G_{11} X = X G_{11}, \quad (G_{11}^T - gI)\alpha^T = 0. \tag{3.13}$$

Note that we are working with a matrix G_{11} which is formed by even supernumbers. In general, we have

$$G_{11} = (G_{11})_0 + \sum_{r=1}^{[N/2]} (G_{11})_{i_1 \cdots i_{2r}} \Theta_{i_1} \cdots \Theta_{i_{2r}}, \tag{3.14}$$

where $(G_{11})_0$, $(G_{11})_{i_1 \cdots i_{2r}}$ are $(n \times n)$-matrices with usual numbers as elements. The orthogonality of G_{11} and the conditions (3.13) imply that $(G_{11})_0 = \epsilon I$ and $g = \epsilon$ with $\epsilon = \pm 1$, while the other matrices $(G_{11})_{i_1 \cdots i_{2r}}$ are antisymmetric and commute with the diagonal matrix X, so that they must be equal to zero. We have thus shown that the simultaneous isotropy group of the *four* solutions U_i is the identity group.

2. Reconstruction

The superposition formula is as usual given by Eq. (2.14), with the supergroup elements to be expressed in terms of the four solutions

$$W_i(t) = \begin{pmatrix} \eta_i(t) \\ Z_i(t) \end{pmatrix} \quad i = 1,\ldots,4, \tag{3.15}$$

with initial conditions corresponding to (3.10). Using the first two solutions and the orthosymplecticity conditions, we obtain

$$\begin{aligned}
&\Gamma_1 = \eta_2 Z_2^{-1} G_{11}, \quad \Gamma_2 = \eta_1 G_{22}, \quad G_{12} = Z_1 G_{22}, \quad G_{21} = Z_2^{-1} G_{11}, \\
&\Lambda_1 = g(\eta_1 - \eta_2 Z_2^{-1} Z_1)(Z_2 - Z_1)^{-1} Z_2, \quad \Lambda_2 = g(\eta_1 - \eta_2)(Z_2 - Z_1)^{-1}, \\
&g = [1 - (\eta_1 - \eta_2 Z_2^{-1} Z_1)(Z_2 - Z_1)^{-1} Z_2 (Z_2 - Z_1)^T (\eta_1 - \eta_2)^T \\
&\quad + (\eta_1 - \eta_2)(Z_2 - Z_1)^{-1} Z_2^T (Z_2 - Z_1)^{-T} (\eta_1 - \eta_2 Z_2^{-1} Z_1)^T]^{-1/2}, \\
&G_{22} = (Z_2 - Z_1 + \eta_2^T \eta_1) Z_2^T G_{11}^{-T}.
\end{aligned} \tag{3.16}$$

With the solutions $W_3(t)$ and $W_4(t)$ we also get two equations from the even part of the conditions $\mathcal{G}W_a(t) = W_a(t)$ $(a = 3,4)$, namely,

$$G_{11} G_{11}^T = Z_2 (Z_2 - Z_3)^{-1} (Z_3 - Z_1)(Z_2 - Z_1 + \eta_2^T \eta_1)^{-1} Z_2^T \equiv N_1(t), \tag{3.17a}$$

$$\begin{aligned}
G_{11} X G_{11}^T = {} & Z_2 (Z_2 - Z_4)^{-1} (Z_4 - Z_1)(Z_2 - Z_1 + \eta_2^T \eta_1)^{-1} Z_2^T + g Z_2 (Z_2 - Z_4)^{-1} \\
& \times [Z_4 (Z_2 - Z_1)^{-T} (\eta_1 - \eta_2)^T - Z_2^T (Z_2 - Z_1)^{-T} (\eta_1 - \eta_2 Z_2^{-1} Z_1)] \alpha G_{11}^T \equiv N_2(t) + N_3(t) g G_{11}^T.
\end{aligned} \tag{3.17b}$$

Equations (3.17) determine G_{11} and g completely in terms of the known quantities N_1, N_2, and N_3 (up to a common sign that we choose to be such that $g(0) = 1$). Indeed if we develop $G_{11}(t)$, $g(t)$, and $N_i(t)$ in (3.17) in terms of the Grassmann basis, as in (2.1) and (2.2), we find that the body of G_{11} is expressed in terms of the eigenvectors and eigenvalues of the bodies of N_1 and N_2. The further coefficients in the expansion of $G_{11}(t)$ are then obtained by successively solving a system of linear algebraic equations.

IV. SUPERPOSITION FORMULA FOR THE EQUATIONS BASED ON OSP(2,2)

The supergroup OSP(2,2) is of dimension $d = (4,4)$. The homogeneous space $\mathrm{OSP}(2,2)/G^0$ is of dimension (1,2) and thus leads to a system (2.13) of one even and two odd ODEs which admits a superposition formula (2.14).

A. Fundamental set of solutions

Let us, with no loss of generality, choose the first solution U_1 in homogeneous coordinates such that its initial value is

$$U_1(0) = (0\ 0\ 1)^T. \tag{4.1}$$

Thus the condition $\mathcal{G}U_1(0) \sim U_1(0)$ implies that $\mathcal{G} = \mathcal{G}_0 \equiv$ (2.7). The constraints (2.8) reduce in this case to the orthogonality of G since the matrices G_{ij} are one dimensional. Following the same reasoning as before we can choose a second solution U_2 such that

$$U_2(0) = (0\ 1\ 0)^T. \tag{4.2}$$

By imposing $\mathcal{G}_0 U_2(0) \sim U_2(0)$ we find the matrix

$$\mathcal{G}_0' = \begin{pmatrix} G & 0 & 0 \\ 0 & g_{11} & 0 \\ 0 & 0 & g_{11}^{-1} \end{pmatrix} \quad \text{with } GG^T = I. \tag{4.3}$$

Thus the isotropy group of the two sets of initial values (4.1) and (4.2) is represented by block diagonal matrices (4.3). To reduce the isotropy group further, we must resort to supplementary solutions with a different type of initial conditions.

Let us choose a solution V such that $V(0)$ is an arbitrary supervector

$$V(0) = (\beta x y)^T, \tag{4.4}$$

with β a nonzero (1×2)-odd supervector and x, y invertible even supernumbers. The condition $\mathscr{G}_0' V(0) \cong V(0)$ implies that $g_{11} = g_{11}^{-1}$, that is $g_{11} = \epsilon$ with $\epsilon = \pm 1$. Moreover, we have to satisfy

$$(G - \epsilon I)\beta^T = 0. \tag{4.5}$$

In general, one equation of the type (4.5) does not imply $G = \epsilon I$. To proceed further we specify the number N of generators in the Grassmann algebra Λ_N.

For $N=1$, G is an orthogonal matrix formed by numbers and β is an odd vector: $\beta = B\Theta$, where $B \in F^{1\times 2}$ ($F = \mathbb{R}$ or $\mathbb{C}$) is a numerical vector. Since G is orthogonal and B is not zero, Eq. (4.5) implies that $G = \epsilon I$. Thus *three* solutions are sufficient to stabilize to the identity transformation.

For $N=2$, we have

$$G = (G)_0 + (G)_{12}\Theta_1\Theta_2, \quad \beta = B_1\Theta_1 + B_2\Theta_2. \tag{4.6}$$

The orthogonality of G implies

$$(G)_0^T(G)_0 = I, \quad (G)_0^T(G)_{12} + (G)_{12}^T(G)_0 = 0 \tag{4.7}$$

and Eq. (4.5) becomes

$$((G)_0 - \epsilon I)B_i^T = 0, \quad i = 1,2. \tag{4.8}$$

From the orthogonality of $(G)_0$, we find $(G)_0 = \epsilon I$ and then $(G)_{12}^T = -(G)_{12}$. Finally, $\mathscr{G}_0' \equiv (4.3)$ takes the form (2.16). Here again *three* solutions are sufficient to stabilize to the identity transformation.

For $N=3$, we can write

$$G = (G)_0 + \sum_{\substack{i,k=1 \\ i<k}}^{3} (G)_{ik}\Theta_i\Theta_k,$$

$$\beta = \sum_{i=1}^{3} B_i\Theta_i + B_{123}\Theta_1\Theta_2\Theta_3. \tag{4.9}$$

The orthogonality conditions are

$$(G)_0^T(G)_0 = I, \tag{4.10a}$$

$$(G)_0^T(G)_{ik} + (G)_{ik}^T(G)_0 = 0, \quad \forall i,k = 1,2,3. \tag{4.10b}$$

Equation (4.5) thus becomes

$$G_0 = \epsilon I, \tag{4.11a}$$

$$(G)_{12}B_3^T + (G)_{23}B_1^T + (G)_{31}B_2^T = 0, \tag{4.11b}$$

with the $(G)_{ik} \in F^{2\times 2}$ antisymmetric matrices characterized by the entries a_{ik}. Equation (4.11b) represents a set of two equations for a_{12}, a_{13}, and a_{23}. In order to force all the quantities a_{ik} to be equal to zero, we need further equations and hence need two solutions $V^{(1)}$ and $V^{(2)}$ of the type (4.4) with $(B_i)^{(a)} = (u_i^{(a)}, v_i^{(a)})$, $i = 1,2,3$, $a = 1,2$. The a_{ik}'s have to then satisfy the set of equations

$$\begin{pmatrix} u_1^{(1)} & u_2^{(1)} & u_3^{(1)} \\ u_1^{(2)} & u_2^{(2)} & u_3^{(2)} \\ v_1^{(1)} & v_2^{(1)} & v_3^{(1)} \\ v_1^{(2)} & v_2^{(2)} & v_3^{(2)} \end{pmatrix} \begin{pmatrix} a_{23} \\ a_{31} \\ a_{12} \end{pmatrix} = 0, \tag{4.12}$$

which implies $a_{ik} = 0$, $\forall i,k$ if and only if three of the four vectors $\mathbf{u}^{(a)}$, $\mathbf{v}^{(a)}$ are linearly independent. Finally, in this case, *four* solutions are required to stabilize to the identity.

For $N = 4$, we have

$$G = (G)_0 + \sum_{i<k} (G)_{ik}\Theta_i\Theta_k + G_{1234}\Theta_1\Theta_2\Theta_3\Theta_4,$$

$$\beta = \sum_i B_i\Theta_i + \sum_{\substack{i,j,k \\ i<j<k}} B_{ijk}\Theta_i\Theta_j\Theta_k. \tag{4.13}$$

The orthogonality of G implies that we have

$$(G)_0^T(G)_0 = I, \tag{4.14a}$$

$$(G)_0^T(G)_{ik} + (G)_{ik}^T(G)_0 = 0, \tag{4.14b}$$

$$\begin{aligned}(G)_0^T(G)_{1234} + (G)_{1234}^T(G)_0 + (G)_{12}^T(G)_{34} \\ + (G)_{34}^T(G)_{12} + (G)_{14}^T(G)_{23} + (G)_{23}^T(G)_{14} \\ - (G)_{13}^T(G)_{24} - (G)_{24}^T(G)_{13} = 0.\end{aligned} \tag{4.14c}$$

Thus Eq. (4.5) becomes

$$(G)_0 = \epsilon I, \tag{4.15a}$$

$$\begin{aligned}(G)_{12}B_3^T + (G)_{23}B_1^T - (G)_{13}B_2^T = 0, \\ (G)_{12}B_4^T + (G)_{24}B_1^T - (G)_{14}B_2^T = 0, \\ (G)_{13}B_4^T + (G)_{34}B_1^T - (G)_{14}B_3^T = 0, \\ (G)_{23}B_4^T + (G)_{34}B_2^T - (G)_{24}B_3^T = 0,\end{aligned} \tag{4.15b}$$

with the (2×2)-antisymmetric matrices $(G)_{ik}$ characterized by the numbers a_{ik}. In principle, we get an overdetermined system (4.15b) of eight equations for six unknowns. But it is easy to show that the system is at most of rank 5. Since we have to prove that all the a_{ik}'s and then the $(G)_{ik}$'s are zero, we must consider two different solutions of the type (4.4) which we call $V^{(1)}$ and $V^{(2)}$. We now obtain a system of 16 equations where the entries of the $B_i^{(a)}$ ($i = 1,\ldots,4$; $a = 1,2$) can be chosen so that it is of rank 6.

Note that all the $(G)_{ik}$'s being equal to zero, we have the additional condition $(G)_{1234}^T = -(G)_{1234}$ following from (4.14c). We thus find the form (2.16) for $\mathscr{G}_0' \equiv (4.3)$ and *four* solutions have been required to reduce the stabilizer to the identity transformation.

From these examples, it is quite clear that the number of particular solutions increases with N. We see that for $N = 1,2$, we need to have $(2+1)$ solutions (2 of type U and 1 of type V) while for $N = 3,4$, we have $(2+2)$ solutions. We conjecture that the number of particular solutions required to stabilize to the identity transformation is equal to $2 + [(N+1)/2]$ when we work in a Grassmann algebra Λ_N.

B. Reconstruction

The reconstruction of the group element $\mathscr{G}(t) \in \mathrm{OSP}(2/2)$ follows exactly along the lines described in Sec. IV A. Indeed, the first two particular solutions U_1 and U_2, with initial conditions (4.1) and (4.2), respectively, and the orthogonality conditions give the following expressions:

$$\begin{aligned}g_{22} &= z_2[z_2 - z_1 + \eta_2^T\eta_1]^{-1}g_{11}^{-1}, \\ g_{12} &= z_1 z_2[z_2 - z_1 + \eta_2^T\eta_1]^{-1}g_{11}^{-1}, \\ g_{21} &= z_2^{-1}g_{11},\end{aligned} \tag{4.16a}$$

$$\begin{aligned}\Gamma_1 &= z_2^{-1}\eta_2 g_{11}, \\ \Gamma_2 &= z_2[z_2 - z_1 + \eta_2^T\eta_1]^{-1}\eta_1 g_{11}^{-1},\end{aligned} \tag{4.16b}$$

$$\Lambda_1 = (z_1 - z_2)^{-1} G^T (z_1 \eta_2 - z_2 \eta_1),$$
$$\Lambda_2 = (z_1 - z_2)^{-1} G^T (\eta_2 - \eta_1), \tag{4.16c}$$

and finally

$$G^T [(z_1 - z_2)^{-1} (z_1 - z_2 + \eta_2 \eta_1^T - \eta_1 \eta_2^T)] G = I. \tag{4.17}$$

In (4.16) and (4.17), $(\eta_i \; z_i)^T$ $(i = 1,2)$ are the components of the two given particular solutions W_1, W_2 in affine coordinates. Note that we see that everything is expressed now in terms of the entry g_{11} and the matrix G.

All the other $[(N+1)/2]$ solutions $V^{(i)} \equiv (4.4)$ will give us the element g_{11} and the matrix entries of G.

V. CONCLUSION

We have shown that the concept of nonlinear ordinary differential equations with superposition formulas can be generalized to superequations. The approach that we generalized was the one based on the transitive primitive action of a Lie group G on a homogeneous space G/G_0, where G_0 is a maximal Lie subgroup of G, not containing an invariant subgroup of G.[2] Replacing G and G_0 by supergroups [in this article $G \sim \mathrm{OSP}(m,2n)$ and G_0 is given in (2.7)] we obtain the system of superequations (2.13). This system has a superposition formula (2.14).

Let us mention that this is not the only path available for extending the concept of nonlinear superposition to superequations. A different possibility is to follow the procedure of Fatyga *et al.*[23] One starts from a system of ODEs that has a superposition formula and views all the entries as Grassmann valued functions. As an example, consider the ordinary Riccati equation

$$\dot{z}(t) = a_1(t) + a_2(t) z + a_3(t) z^2, \tag{5.1}$$

where $z(t)$ and $a_i(t)$ $(i = 1,2,3)$ are Grassmann valued functions. Splitting each of them into even and odd parts

$$z = w + \eta, \quad a_i = r_i + \alpha_i, \tag{5.2}$$

we obtain the system

$$\dot{w} = r_1 + r_2 w + \alpha_2 \eta + r_3 w^2 + 2\alpha_3 w\eta,$$
$$\dot{\eta} = \alpha_1 + r_2 \eta + \alpha_2 w + 2r_3 w\eta + \alpha_3 w^2. \tag{5.3}$$

The system (5.3) is not of the type considered in this article, although it does inherit a superposition formula from the Riccati equation (5.1), namely

$$z = [z_2 (z_3 - z_1) c - z_1 (z_3 - z_2)] / [(z_3 - z_1) c - (z_3 - z_2)]. \tag{5.4}$$

A study of the relationship between the two types of generalizations goes beyond the scope of the present article.

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An analytic solution to the Thomas–Fermi equation

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A perturbative procedure due to Bender *et al.* (here referred to as the BMPS procedure) [J. Math. Phys. **30**, 1447 (1989)] and useful in solving difficult nonlinear problems, has been used here to solve the Thomas–Fermi (T–F) equation. The present work attempts to balance the ease of the ensuing analysis with the use of an analytic, zero-order function that already contains a good deal of the nonlinearity of the T–F equation. The initial slope of the T–F potential is computed with 0.35% error in a second-order application of the theory.

I. INTRODUCTION

Recently, Bender *et al.*[1] (BMPS) have proposed a new approach to the analytic solution of nonlinear problems in mathematics and physics. Application of the method to nonlinear differential equations such as the Thomas–Fermi (T–F) equation,

$$\Phi''(x) = \Phi^{3/2}(x)/\sqrt{x}, \quad \Phi(0) = 1, \quad \Phi(\infty) = 0, \tag{1.1}$$

might be especially far reaching. In this case, the BMPS procedure has consisted of replacing the right-hand side of the T–F equation by one which contains the parameter δ, i.e.,

$$\Phi''(x) = \Phi \cdot (\Phi/x)^{\delta}. \tag{1.2}$$

The potential Φ is then expanded in a power series in δ

$$\Phi = \Phi_0 + \delta\Phi_1 + \delta^2\Phi_2 + \cdots. \tag{1.3}$$

This, in turn, produces a set of linear equations for the Φ_n functions:

$$\Phi''_0 - \Phi_0 = 0,$$

$$\Phi''_1 - \Phi_1 = \Phi_0 \ln(\Phi_0/x),$$

$$\Phi''_2 - \Phi_2 = \Phi_1\left[1 + \ln\frac{\Phi_0}{x}\right] + \frac{1}{2}\Phi_0 \ln^2\frac{\Phi_0}{x},$$

$$\cdots$$

with associated boundary conditions $\Phi_0(0) = 1, \Phi_0(\infty) = 0$, and $\Phi_n(0) = \Phi_n(\infty) = 0$ for $n > 1$. The appropriate solution of the zero-order problem being

$$\Phi_0 = e^{-x}.$$

Solutions for the higher-order functions can be obtained by quadratures and a solution to the T–F equation is recovered by setting $\delta = (1/2)$ in Eq. (1.3). For example, Φ_1 is given by (γ is Euler's constant)

$$\Phi_1 = \tfrac{1}{4}e^{-x}\{\gamma + \ln(2) - x + x^2 + (1 + 2x)\ln(x) - e^{2x}\,\mathrm{Ei}(-2x)\}.$$

Additional higher-order functions are also obtainable but complicated.

One measure of the rapidity of convergence of the procedure is provided by calculations of the value of the initial slope $\Phi'(0)$ of the T–F potential. This quantity, difficult to compute by any means, plays an important role in determining many of the physical properties of the Thomas–Fermi atom. For example, the energy (in atomic units) for a neutral atom of atomic number Z is

$$E = \tfrac{6}{7}(4/3\pi)^{2/3}Z^{7/3}\Phi'(0).$$

A highly accurate numerical solution of the T–F equation has been provided by Kobayashi *et al.*[2] who give the initial slope $\Phi'(0)$ as $-1.588\,071\,0$. Given the nonlinearity of the T–F equation and the global nature of its boundary conditions some 25 years passed from its inception until the slope was known to seven figures. Within the BMPS approach and with the choice made by Bender *et al.* in Eq. (1.2), the computed initial slope at zero order is found to be in 36% error. At first, second, and third order the slope contains 25%, 13%, and 6.9% error, respectively. Bender was able to improve his estimate of the initial slope to a 1.1% error by expressing Eq. (1.3) as a [2,1] Padé approximant with $\delta = (1/2)$.

II. AN ALTERNATE ANALYTIC T–F POTENTIAL

In this paper we wish to point out that the BMPS approach is capable of much more rapid convergence near the origin if we include some of the nonlinearity for the full T–F equation in the zero-order function. We do this by replacing the T–F equation with

$$\Phi'' = (\Phi/\sqrt{x})\Phi^{\delta}. \tag{2.1}$$

That is, we start with a $\sqrt{x}$ containing, but still analytic, zero-order problem and gradually add the remaining nonlinearity at higher order. Representing Φ by the series in Eq. (1.3) we get as before a sequence of inhomogeneous equations for the perturbation functions Φ_n (boundary conditions as before)

$$\Phi''_n - \Phi_n/\sqrt{x} = R_n(x)/\sqrt{x}. \tag{2.2}$$

The first few inhomogeneous terms being given by

$$R_0 = 0,$$

$$R_1 = \Phi_0 \ln \Phi_0,$$

$$R_2 = \Phi_1[1 + \ln \Phi_0] + \tfrac{1}{2}\Phi_0 \ln^2 \Phi_0,$$

$$R_3 = \Phi_2[1 + \ln \Phi_0] + \frac{1}{2}\frac{\Phi_1^2}{\Phi_0} + \Phi_1\left[1 + \frac{1}{2}\ln \Phi_0\right] \times \ln \Phi_0 + \frac{1}{6}\Phi_0 \ln^3 \Phi_0.$$

Two linearly independent solutions for the zero-order equa-

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tion are immediately obtainable in terms of modified Bessel functions[3] K_ν and I_ν with fractional order ν, i.e.,

$$f(x) = \frac{2}{\Gamma(2/3)}\left(\frac{2}{3}\right)^{2/3}\sqrt{x}K_{2/3}(\zeta),$$
$$g(x) = \Gamma\left(\frac{2}{3}\right)\left(\frac{2}{3}\right)^{1/3}\sqrt{x}I_{2/3}(\zeta), \tag{2.3}$$

where the argument ζ is $(4/3)x^{3/4}$. We note that Φ_0 is $f(x)$ since it satisfies the boundary conditions at zero and infinity. Construction of the Green's function for the operator in Eqs. (2.2) is straightforward and the general solution of those equations are

$$\Phi_n(x) = -f(x)\int_0^x g(s)R_n(s)\frac{ds}{\sqrt{s}} - g(x)\int_x^\infty f(s)R_n(s)\frac{ds}{\sqrt{s}}. \tag{2.4}$$

The initial slopes of the potential functions Φ_n follow from Eq. (2.4) and we obtain

$$\Phi'_n(0) = -\int_0^\infty f(s)R_n(s)\frac{ds}{\sqrt{s}}. \tag{2.5}$$

III. NUMERICAL RESULTS

In this section some comparisons will be made between the numerical solution[2] to the T–F equation and the one obtained here. The present calculations are facilitated by noting that the modified Bessel functions encountered above are related to the Airy functions[3,4] Ai(z), Bi(z), and their derivatives Ai'(z) and Bi'(z). We have

$$f(x) = \Phi_0(x) = A(z),$$
$$g(x) = \frac{1}{2}\left(\frac{3}{2}\right)^{1/3}\frac{\Gamma(2/3)}{\Gamma(1/3)}[B(z) - A(z)], \tag{3.1}$$

where $A(z) = \mathrm{Ai}'(z)/\mathrm{Ai}'(0)$, $B = \mathrm{Bi}'(z)/\mathrm{Bi}'(0)$, and $z = 2^{2/3}\sqrt{x}$. The Airy functions satisfy the equation $w'' = zw(z)$ and have the initial values:

$$\mathrm{Ai}(0) = \mathrm{Bi}(0)/\sqrt{3} = [3^{2/3}\Gamma(2/3)]^{-1} = 0.355\,028\,053\,8,$$
$$-\mathrm{Ai}'(0) = \mathrm{Bi}'(0)/\sqrt{3} = [3^{1/3}\Gamma(1/3)]^{-1} = 0.258\,819\,403\,7. \tag{3.2}$$

The initial slope of the zero-order function consequently is just

$$\Phi'_0(0) = -\left(\frac{2}{3}\right)^{1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)} = -1.728\,260\,4.$$

This is a good first approximation but too negative by about 8%. The first-order slope is given by

$$\Phi'_1(0) = -2^{1/3}\int_0^\infty A^2(z)\ln[A(z)]dz. \tag{3.3}$$

Analytic evaluation of this integral and the ones that follow does not appear to be possible. However, there is some hope (cf. the Appendix) that progress can be made in that direction if further work is done in this somewhat neglected area of special function theory. Numerical evaluation of the integral in Eq. (3.3) yields a value of 0.332 226 0 and

$$\tfrac{1}{2}\Phi'_1(0) = +0.166\,113\,0.$$

To first order, the initial T–F slope is $-1.562\,147\,4$ with an error of 1.63%. Evaluation of the second-order, initial slope requires evaluation of integrals of the sort

$$\Phi'_2(0) = -\frac{1}{2}\int_0^\infty [f(s)\ln f(s)]^2\frac{ds}{\sqrt{s}} - \int_0^\infty f(s)[1 + \ln f(s)]\Phi_1(s)\frac{ds}{\sqrt{s}}.$$

With the help of Eqs. (2.4) and (3.1) these become

$$\Phi'_2(0) = -\left(\frac{1}{2}\right)^{2/3}\int_0^\infty [A(z)\ln A(z)]^2 dz + \left(\frac{3}{4}\right)^{1/3}\frac{\Gamma(2/3)}{\Gamma(1/3)} \times \int_0^\infty\int_0^z A^2(z)A(z')[B(z') - A(z')] \times [\ln\{A(z)A(z')\} + 2\ln A(z)\ln A(z')]dz'\,dz,$$

where we have inverted the order of integration in the integral representing Φ_1. The magnitudes of these integrals have also been obtained numerically. The first has a value of 0.213 390 and the second 0.018 819. As a result

$$\tfrac{1}{4}\Phi'_2(0) = -0.031\,446.$$

Thus the initial slope of the T–F potential to second order is $-1.593\,593$, i.e., an error of 0.35%. We see that the corrections are causing the slope to oscillate about the "exact" value with rapidly decreasing amplitude. This estimate of the initial slope can be further improved if, following Bender we convert Eq. (1.3) to a [1,1] Padé approximant and evaluate this at $\delta = (1/2)$. This results in an initial slope of $-1.588\,588$, i.e., an error of 0.03%.

Encouraged by our estimates of the initial slope of the T–F potential we have also made a comparison (to first order) of the numerical solution for $\Phi(x)$ with the "analytical" results obtained in this work. Higher-order calculations are certainly possible. We see in Fig. 1 that there is fairly good agreement (less than 5% error) between the two curves for x values less than 4 units. At larger distances the analytic solution drops off more rapidly than the exact one. This is to be expected since the Airy function Ai'(z) decreases exponentially for large x whereas the exact solution is known to vary as x^{-3} in that range. Whether this situation is correctable at higher order is not clear at this point since a proper asymptotic analysis of the Φ_n functions has not been made. Progress along those lines will depend on a deeper knowledge of the properties of Airy functions than is presently available.

In summary, a judicious choice of the nonlinear term in the T–F equation together with the BMPS method has produced a rapidly converging analytic solution to that equation near the origin. At larger distances (the midphysical range) corrections higher than first order are needed to obtain accurate values of the potential. Although the theory is perfectly amenable to numerical solution, it would be highly desirable to have an analytic representation for the potential at those distances. Some progress along that path might be possible as indicated in the Appendix.

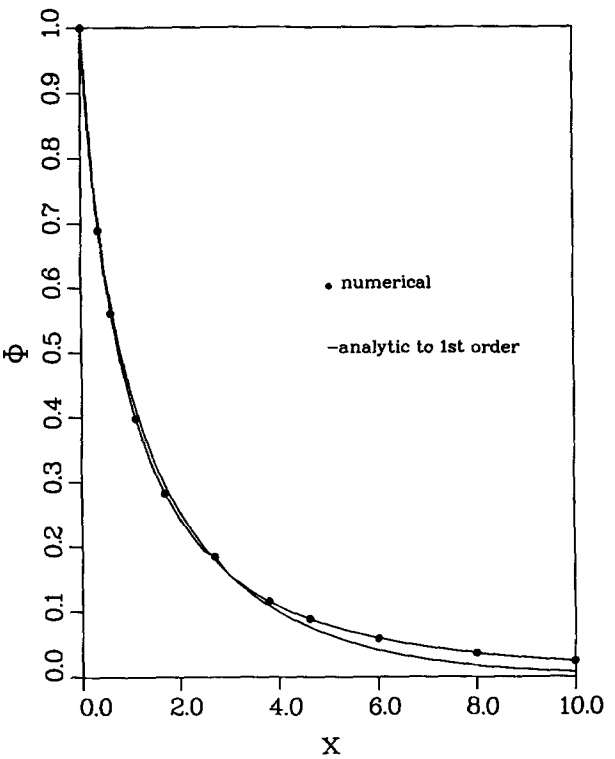

FIG. 1. Numerical and analytic (first-order) solutions of the Thomas–Fermi equation.

APPENDIX: INTEGRALS OF AIRY FUNCTIONS

The existing literature on the integrals of Airy functions is quite small. However, there have been some recent contributions[5,6] in that area. Here, we wish to note some additional results that might allow the analysis begun in this paper to progress. We start by noting the elementary results:

$$\int \mathrm{Ai}^2(x)dx = x\,\mathrm{Ai}^2(x) - \mathrm{Ai}'^2(x),$$

$$\int \mathrm{Ai}'^2(x)dx = \frac{1}{3}\{x\,\mathrm{Ai}'^2(x) - x^2\,\mathrm{Ai}^2(x) + 2\,\mathrm{Ai}(x)\mathrm{Ai}'(x)\}.$$

Higher moment integrals of these Airy functions can also be obtained in closed form. If we define the functions $F_n(x)$, and $G_n(x)$ by

$$F_n(x) = \int x^n\,\mathrm{Ai}^2(x)dx,$$

$$G_n(x) = \int x^{n-1}\,\mathrm{Ai}'^2(x)dx,$$

then integration by parts for each of this pair of functions produces the recurrence relations:

$$(2n+1)F_n(x) = \tfrac{1}{2}n(n-1)(n-2)F_{n-3}(x) + nx^{n-1}\,\mathrm{Ai}(x)\mathrm{Ai}'(x) - x^n\,\mathrm{Ai}'^2(x) + x^{n-2}\,\mathrm{Ai}^2(x)[x^3 - n(n-1)/2],$$

$$nG_n(x) = x^n\{\mathrm{Ai}'^2(x) - x\,\mathrm{Ai}^2(x)\} + (n+1)F_n(x). \tag{A1}$$

We will denote values of the corresponding definite integrals over the interval $0 \leqslant x \leqslant \infty$ by $\mathbf{F}_n$ and $\mathbf{G}_n$. Using the results given above, together with the limiting values[3] of the Airy functions we find

$$\mathbf{F}_0 = \left[3^{1/3}\Gamma\left(\frac{1}{3}\right)\right]^{-2}, \quad \mathbf{F}_1 = \frac{\sqrt{3}}{18\pi},$$

$$\mathbf{F}_2 = \frac{1}{5}\left[3^{2/3}\Gamma\left(\frac{2}{3}\right)\right]^{-2},$$

and the useful difference equations:

$$(4n+2)\mathbf{F}_n/n! = \mathbf{F}_{n-3}/(n-3)!, \quad n\mathbf{G}_n = (n+1)\mathbf{F}_n.$$

The solution of these equations is not difficult and we have for general n:

$$\mathbf{F}_n = \frac{\Gamma(n+1)\Gamma(7/6)}{\Gamma(n/3+7/6)12^{n/3}}\mathbf{F}_0,$$

$$\mathbf{G}_n = \frac{\Gamma(n+2)\Gamma(7/6)}{n\Gamma(n/3+7/6)12^{n/3}}\mathbf{F}_0. \tag{A2}$$

Applying these exact results to the problems in this paper is not completely possible as we shall see below. For example, if the integral in Eq. (3.3) is integrated by parts we find [with the help of Eq. (A2)] that

$$\int_0^\infty \mathrm{Ai}'^2(z)\ln\frac{\mathrm{Ai}'(z)}{\mathrm{Ai}'(0)}dz = -\frac{\sqrt{3}}{54\pi} + \frac{1}{3}\int_0^\infty \frac{z^3\,\mathrm{Ai}^3(z)dz}{\mathrm{Ai}'(z)}.$$

Expansion of the ratio Ai/Ai' in powers of z followed by term-by-term integration using Eq. (A2) yields a slowly converging series that is virtually useless. A further integration by parts, however, gives

$$-\frac{\sqrt{3}}{27\pi} + \frac{1}{12}\int_0^\infty \frac{z^5\,\mathrm{Ai}^4(z)dz}{\mathrm{Ai}'^2(z)},$$

where the integral term is fairly small. A final integration by parts yields the approximation,

$$\int_0^\infty \frac{z^5\mathrm{Ai}^4(z)dz}{\mathrm{Ai}'^2(z)} \approx \frac{11\Gamma(1/3)^6}{96\pi^4} - \frac{13\sqrt{3}}{18\pi}.$$

As a result, the integral in Eq. (3.3) is roughly given by

$$\int_0^\infty A(z)^2\ln A(z)dz \approx -\frac{7}{12}C + \frac{11}{72}C^4, \tag{A3}$$

where $C = \Gamma(1/3)/3^{1/3}\Gamma(2/3)$. Within this degree of approximation, the computed value of the integral in question is -0.2593 whereas the value obtained by numerical integration is -0.2637. The right-hand side of Eq. (A3) however, might be regarded as part of an asymptotic represention of the integral and therefore capable of refinement.

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