Geometry of homothetic Killing trajectories and stationary limit surfaces

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We investigate the intrinsic geometry of timelike and null homothetic Killing trajectories. We do this through the use of two different Frenet–Serret formalisms developed by Synge and Bonnor. The curvature of such a nongeodesic timelike curve passing through a spacetime point is a direct measure of the expansion of the congruence at that point. Moreover, the rotation of this congruence is directly related to the torsions of its individual curves. For both classes of curves, timelike and null, the intrinsic scalars can be expressed as exponential functions of suitable parameters. We prove the following theorem twice, first by using the timelike formalism, and then through the null one. A homothetic stationary limit surface (where the homothetic Killing vector becomes null) is a null geodesic hypersurface if and only if the rotation of the homothetic Killing congruence vanishes on that hypersurface. The second, "null" approach allows us to derive this theorem directly on the hypersurface. Finally, we note that by setting a parameter equal to zero we recover all of the corresponding results for ordinary Killing vectors.

1. INTRODUCTION

The concept of a Killing horizon, a familiar idea in black hole physics, was first developed when Carter[1] and Vishveshwara[2] independently considered asymptotically flat spacetimes admitting a time translational Killing vector (KV). Their analysis led to the result that a static limit surface (where the KV becomes null) is a null geodesic hypersurface if and only if the rotation of the Killing congruence vanishes on that hypersurface. The same result was later obtained in an entirely different manner from the original approach.[3] In particular it was derived by first using a Frenet–Serret formalism for timelike Killing curves, and then taking a limit onto a static limit surface where this formalism breaks down. This approach is valid because each of the relevant terms involved in the theorem is both independent of the formalism and well defined on the hypersurface. However, it also suggests examining the trajectories, through other means, directly on the hypersurface.

If we assume that spacetime admits a homothetic Killing vector (HKV), ξ^a, then the metric can be written in the form $g_{ab}=e^{c\tau}h_{ab}$ where c is a constant, τ is a parameter along the trajectory, and h_{ab} is a function on the spacetime with the restriction that it be constant along any particular HK trajectory.[4] For a KV c is zero. It follows that an HK observer experiences a homothetic change in g_{ab} as he moves along his trajectory. Furthermore, if the HK congruence is irrotational, he concludes that the spacetime is "homothetically static"; otherwise he concludes that the spacetime is "homothetically stationary." In regions where the HKV is not timelike, such an observer cannot exist. We therefore term the boundary, where the HKV becomes null, to be a "homothetic stationary limit surface." It would seem appropriate to distinguish between static and stationary limit surfaces even for spacetimes having an ordinary KV.

More recently,[5] some of the earlier results for KV's have been extended to spacetimes admitting a timelike conformal Killing vector (CKV). For example, the "conformal stationary limit surface" is introduced, and shown to be an infinite frequency shift surface for CK sources and observers. Moreover, the necessary and sufficient conditions for this hypersurface to be null and geodesic were given, having relevance to the existence of horizons in such spacetimes.

In this paper we study the intrinsic geometry of both timelike and null nongeodesic HK congruences. We do this via two different Frenet–Serret formalisms developed by Synge[6,7] and Bonnor.[8] This allows us to (a) consider the geometry of timelike HK trajectories that are infinitesimally close to a homothetic stationary limit surface and (b) consider the geometry of these trajectories when they degenerate into null HK curves on the hypersurface itself. Furthermore, we can readily obtain the geometry of ordinary Killing trajectories from these results. This includes the case of time-translational Killing curves in Kerr spacetime. These are nongeodesic and timelike outside the stationary limit surface but nongeodesic and null on it.

2. TIMELIKE HOMOTHETIC KILLING TRAJECTORIES

Consider a spacetime that admits a homothetic Killing vector ξ^a. Such a vector satisfies[4]

$$\pounds_\xi g_{ab}\equiv\nabla_a\xi_b+\nabla_b\xi_a=2\phi g_{ab}, \tag{1}$$

where $\pounds_\xi$ is the Lie derivative along ξ, ϕ is a constant scalar defined by $\phi=\frac{1}{4}\nabla_a\xi^a$, g_{ab} is the metric tensor, and ∇_a is its associated covariant derivative operator. We adopt the convention that Latin indices range and sum from 0 to 3, while Greek indices range and sum from 1 to 3, and we choose a signature of -2. If $\phi=0$, then ξ^a is an ordinary Killing vector corresponding to an isometry of the spacetime. For the present we shall assume that ξ^a is timelike in which case we can define

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a 4-velocity along ξ^a, viz,

$$u^a = e^{-\psi}\xi^a, \quad \xi^a\xi_a = e^{2\psi}. \tag{2}$$

It is a straightforward task to show that such a congruence is shear-free[9] and has an expansion $\theta \equiv \frac{1}{3}\nabla_a u^a = u^a\nabla_a\psi = \phi e^{-\psi}$.

Since we are interested in studying the properties of such a congruence via the intrinsic geometry of the individual curves, we briefly review the Frenet–Serret (F–S) formalism for timelike curves.[6]

Let $x^a = x^a(s)$ be an arbitrary timelike curve of class C^5 with arc length s. Associated with each point of this curve is the F–S tetrad comprising the unit tangent vector $u^a = dx^a/ds$, and three mutually orthogonal, unit spacelike vectors $e^{\ a}_{(\mu)}$, $\mu = 1, 2, 3$, each of which is orthogonal to u^a. These vectors obey the F–S equations,

$$\begin{bmatrix} \dot{u}^a \\ \dot{e}^{\ a}_{(1)} \\ \dot{e}^{\ a}_{(2)} \\ \dot{e}^{\ a}_{(3)} \end{bmatrix} = \begin{bmatrix} 0 & \kappa & 0 & 0 \\ \kappa & 0 & \tau_1 & 0 \\ 0 & -\tau_1 & 0 & \tau_2 \\ 0 & 0 & -\tau_2 & 0 \end{bmatrix} \begin{bmatrix} u^a \\ e^{\ a}_{(1)} \\ e^{\ a}_{(2)} \\ e^{\ a}_{(3)} \end{bmatrix}, \tag{3a}$$

(3b)

(3c)

(3d)

where $\dot{} \equiv u^b\nabla_b$ is the covariant total derivative operator along the curve and $u^a u_a = 1$, $e^{\ a}_{(\mu)}\, e_{(\nu)a} = -\delta_{\mu\nu}$, and $u^a e_{(\nu)a} = 0$. The scalar coefficients, i.e., the curvature κ and the first and second torsions τ_1 and τ_2, form a complete set of invariants of the curve in spacetime. We choose the sign of κ and τ_1 as positive. The sign of τ_2 is then fixed by imposing a definite handedness, say right-handedness, to the spacelike triad, which is equivalent to assuming that spacetime is orientable. We shall apply the above formalism to timelike HK congruences, i.e., where $u^a = e^{-\psi}\xi^a$ and ξ^a satisfies Eq. (1).

Suppose first that $\kappa = 0$ so that we are dealing with a timelike geodesic. Now $\dot{u}^a = 0$ implies that $\xi^{a'} = h\xi^a$ where $' \equiv \xi^b\nabla_b$ and h is a scalar coefficient. If we transvect the above with ξ_a and make use of the HK equation (1), we find that $0 = \xi^a\xi_a(h - \phi)$. The latter by itself implies that either ξ^a is necessarily null or else $h = \phi$ and ξ^a is not necessarily null. At this point we are only concerning ourselves with timelike trajectories, and so we must have $h = \phi$ whenever $\kappa = 0$. An example of this comes from Minkowski spacetime which admits the HK vector $\xi^a = (t, x, y, z)$. Here $h = \phi = 1$ while ξ^a only becomes null on the light cone.

Suppose now that $\kappa \neq 0$, i.e., we are dealing with non-geodesic HK trajectories. Then we find it useful to use the HK equation (1) to express the acceleration vector as

$$\dot{u}^a = F^{ab}u_b, \quad \text{where } F_{ab} = e^{-\psi}[\phi g_{ab} - \nabla_a\xi_b] = -e^{-\psi}\nabla_{[a}\xi_{b]}. \tag{4}$$

Thus F^{ab} is a second rank antisymmetric tensor. The first of the F–S equations (3a) together with Eq. (4) yields $\kappa e^{\ a}_{(1)} = F^{ab}u_b$. We take the total derivative of this with respect to the arc length s and make use of Eq. (3a) again so that

$$\dot{\kappa}e^{\ a}_{(1)} + \kappa\dot{e}^{\ a}_{(1)} = \dot{F}^{ab}u_b + \kappa F^{ab}e_{(1)b}. \tag{5}$$

At this point we must evaluate $\dot{F}^{ab}$:

$$\dot{F}^{ab} = -\dot{\psi}F^{ab} + e^{-2\psi}\xi^c\nabla_c\nabla^{[b}\xi^{a]}. \tag{6}$$

The last term can be shown to vanish by making use of an identity that is valid for both HKV's as well as ordinary KV's, namely,

$$\nabla_c\nabla_b\xi_a = R_{dcba}\xi^d. \tag{7}$$

(The corresponding identity for CKV's is slightly more complicated.[5] The manner of derivation is the same for KV's, HKV's, and CKV's.) It follows that $\dot{F}^{ab} = -\dot{\psi}F^{ab}$, from which $e^{\psi}F^{ab}$ is constant along the trajectory. Equation (5), with the help of Eq. (4), then reduces to

$$\dot{\kappa}e^{\ a}_{(1)} + \kappa\dot{e}^{\ a}_{(1)} = -\dot{\psi}\kappa e^{\ a}_{(1)} + \kappa F^{ab}e_{(1)b}. \tag{8}$$

If we transvect Eq. (8) with $e_{(1)a}$, we find that

$$-\dot{\kappa} = \dot{\psi}\kappa \quad \text{and} \quad \dot{e}^{\ a}_{(1)} = F^{ab}e_{(1)b}, \tag{9}$$

where we have made use of the fact that F^{ab} is antisymmetric and $e^{\ a}_{(1)}\, e_{(1)a} = -1$ implies that $\dot{e}^{\ a}_{(1)}\, e_{(1)a} = 0$. Now $\theta = \dot{\psi} = e^{-\psi}\phi$ together with $\phi = \text{const}$ leads to $\dot{\theta} = -\theta^2$ so that $(\kappa/\theta)^{\cdot} = 0$. Again, the second F–S equation (3b) together with Eq. (9) yields

$$\kappa u^a + \tau_1 e^{\ a}_{(2)} = F^{ab}e_{(1)b}. \tag{10}$$

If we differentiate Eq. (10) and continue the previous process, we eventually arrive at

$$\dot{\kappa}/\kappa = \dot{\tau}_1/\tau_1 = \dot{\tau}_2/\tau_2 = -\dot{\psi} = -\theta, \quad \dot{\theta} = -\theta^2, \tag{11}$$

or equivalently

$$(\kappa/\theta)^{\cdot} = (\tau_1/\theta)^{\cdot} = (\tau_2/\theta)^{\cdot} = 0. \tag{12}$$

Thus κ/θ, τ_1/θ, and τ_2/θ are constants of the motion. Moreover,

$$\dot{e}^{\ a}_{(\mu)} = F^{ab}e_{(\mu)b}, \quad \mu = 1, 2, 3. \tag{13}$$

There are two solutions to $\dot{\theta} = -\theta^2$, namely $\theta = 0$, and $\theta = (s - a)^{-1}$, where a is a constant, in which case $e^{\psi} = \phi(s - a)$. It is clear that in the second instance these timelike trajectories must always have either $s > a$ or $s < a$ since $e^{\psi} = 0$ corresponds to a null HK vector. On the other hand, the solution $\theta = 0$ corresponds to ordinary Killing trajectories, i.e., $\phi = 0$. Equation (11) then reduces to a previously derived result,[3] namely that κ, τ_1, and τ_2 are constants. Since an HK congruence has $\theta \neq 0$, we see from the above that the curvature of the individual trajectories is a direct measure of the congruence's expansion. We note, however, that an HK congruence can be comprised of geodesics. Our previous example from Minkowski space illustrates this point. For $\xi^a = x^a$ with $x^a x_a > 0$ we have that $\theta = 1/\sqrt{x^a x_a} > 0$ while $\kappa = 0$.

It follows directly from Eq. (11) and $(e^{\psi})^{\cdot} = \phi = \text{const}$ that

$$\frac{\kappa}{\kappa_0} = \frac{\tau_1}{\tau_{10}} = \frac{\tau_2}{\tau_{20}} = \frac{e^{\psi_0}}{e^{\psi}} = \frac{1}{1 + \theta_0 s}, \tag{14}$$

where the point $s = 0$ and the subscript "0" correspond to an arbitrary reference point on the trajectory. Thus all three scalars decrease monotonically as s increases for $\phi = e^{\psi_0}\theta_0 > 0$. It should be noted that $1 + \theta_0 s = 0$ only if $e^{\psi} = 0$. In this instance κ, τ_1, and τ_2 are not defined. This is due to the fact that the F–S formalism that we

have been using until now is specifically geared to timelike curves whereas when $e^{\psi}=0$ the curves are null and u^a is not defined. (We shall deal with the null case later in this paper). We also note that if the curvature vanishes at some point, say $\kappa_0=0$, then $\kappa=0$ everywhere and the curve is a timelike geodesic. (The F–S process is essentially a Gram–Schmidt orthogonalization process along the curve, and it stops when one of the invariants is zero. The rest are usually set equal to zero).

We gain further insight into the significance of the F–S scalars and vectors by operating on u^b with both sides of the bivector identity[10]

$$0=(F^4)^a{}_b-\alpha(F^2)^a{}_b-\beta^2\delta^a{}_b. \tag{15}$$

Here $\alpha=-\frac{1}{2}F^{cd}F_{cd}$, $\beta=-\frac{1}{4}F^{cd}\hat{F}_{cd}$, $\hat{F}_{cd}=\frac{1}{2}\eta_{cdkl}F^{kl}$ is the dual of F_{cd} with η_{cdkl} the alternating tensor, and $(F^n)^a{}_b=F^a{}_kF^k{}_l\cdots F^t{}_b$, $F^a{}_b$ being repeated n times. By repeatedly making use of Eqs. (4), (13), and (3) we arrive at

$$0=[\kappa^2(\kappa^2-\tau_1^2-\alpha)-\beta^2]u^a+\kappa\tau_1[(\kappa^2-\tau_1^2-\tau_2^2)-\alpha]e^{\ a}_{(2)}. \tag{16}$$

This requires that

$$\alpha=\kappa^2-\tau_1^2-\tau_2^2 \quad \text{and} \quad \beta^2=\kappa^2\tau_2^2. \tag{17}$$

We choose the negative square root, i.e.,

$$\beta=-\kappa\tau_2 \tag{18}$$

to conform with an earlier choice for Killing congruences.[11]

Now we examine the rotation vector ω^a of the congruence, i.e.,

$$\omega^a=\tfrac{1}{2}\eta^{abcd}u_b\nabla_c u_d \tag{19}$$

and its associated renormalized vector $\bar{\omega}^a$

$$\bar{\omega}^a=\tfrac{1}{2}\eta^{abcd}\xi_b\nabla_c\xi_d. \tag{20}$$

It follows directly that $\bar{\omega}^a=e^{2\psi}\omega^a$. In view of Eq. (4) we can write these as

$$\bar{\omega}^a=-e^{2\psi}\hat{F}^{ab}u_b=e^{2\psi}\omega^a, \tag{21}$$

where $\hat{F}^{ab}$ is the dual of F^{ab}. From the bivector identity[10]

$$0=(F^3)^{ab}-\alpha F^{ab}-\beta\hat{F}^{ab} \tag{22}$$

it follows that

$$\beta\bar{\omega}^a=e^{2\psi}[\alpha F^{ab}u_b-(F^3)^{ab}u_b]. \tag{23}$$

Again the combined use of Eqs. (4), (13), (3), and (18) simplifies this expression to read[12]

$$\bar{\omega}^a=e^{2\psi}[\tau_2e^{\ a}_{(1)}+\tau_1e^{\ a}_{(3)}]. \tag{24}$$

Equations (24) and (17) then yield

$$\bar{\omega}^a\bar{\omega}_a=-e^{4\psi}[\tau_1^2+\tau_2^2]=e^{4\psi}[\alpha-\kappa^2]. \tag{25}$$

Furthermore, Eqs. (4) and (1) lead to

$$\alpha=-\tfrac{1}{2}F^{cd}F_{cd}=e^{-2\psi}(2\phi^2-\tfrac{1}{2}\nabla^c\xi^d\nabla_c\xi_d). \tag{26}$$

In order to gain further insight into some of the above results, we consider $\xi^a\xi_a=\text{const}$ hypersurfaces. The normal to such a hypersurface is given by

$$n_a=\tfrac{1}{2}\nabla_a(\xi^b\xi_b)=\xi^b\nabla_a\xi_b. \tag{27}$$

With the help of Eqs. (1) and (3a) we can write this as

$$n_a=e^{\psi}[\phi u_a-e^{\psi}\kappa e_{(1)a}], \quad n^an_a=e^{2\psi}[\phi^2-e^{2\psi}\kappa^2]. \tag{28}$$

Finally we combine Eqs. (25), (26), and (28) and find that

$$\bar{\omega}^a\bar{\omega}_a-n^an_a=(\xi^a\xi_a)\,[\phi^2-\tfrac{1}{2}\nabla^c\xi^d\nabla_c\xi_d]. \tag{29}$$

This is a generalization of a well-known theorem for Killing congruences alluded to in the Introduction. It states that a $\xi^a\xi_a=0$ hypersurface, i.e., a homothetic stationary limit surface is a null hypersurface if and only if the rotation vector $\bar{\omega}^a$ vanishes or is null on that hypersurface. When $\phi=0$, we have an ordinary Killing congruence, and Eq. (29) reduces to a well-known equation.[1,2,3] In fact, Eq. (29) is not limited to HK congruences. It is also valid for conformal Killing congruences where $\phi=\frac{1}{4}\nabla_a\xi^a$ is a function of spacetime position. This and the full implications of this equation are discussed in greater detail elsewhere.[5] We note at this point that while Eq. (29) was derived here via a formalism that is valid only for timelike curves, each of its terms as defined through Eqs. (20), (27), and (1) is well defined when ξ^a becomes null. Hence Eq. (29) is valid on a homothetic stationary limit surface. We shall derive this equation directly on such a hypersurface in the following section when we consider nongeodesic null HK congruences.

3. NULL HOMOTEHETIC KILLING TRAJECTORIES

The geometry of nongeodesic null curves in spacetime was first considered by Bonnor.[8] Though his study was restricted to real null curves in Minkowski space, he noted that many of his results could be generalized to curved Riemannian spacetimes. He encountered an interesting problem in his study of these curves, namely the absence of a simple parameter corresponding to the proper time of a timelike line, or the affine parameter of a null geodesic. He overcame this difficulty by introducing a pseudo-arc that is defined invariantly with respect to parameter transformations. Synge,[7] in a later study, sidestepped and simplified this problem by restricting himself to dynamical nongeodesic null lines corresponding to a massless particle with a *given* 4-momentum p^a tangent to the curve. While the physical reality of such a hypothetical particle is not clear, his assumption does ensure the existence of a unique special parameter λ such that $p^a=dx^a/d\lambda$. Now we shall concern ourselves with nongeodesic null HK trajectories, i.e., curves whose null tangent vector ξ^a satisfies the HK equation (1). It follows that there exists a unique special parameter λ such that $\xi^a=dx^a/d\lambda$. Since our approach is analogous to Synge's, we shall proceed along his mathematical lines and use the Frenet–Serret equations that he develops.

Let $x^a=x^a(\lambda)$ be a nongeodesic null curve with a given tangent vector ξ^a such that $\xi^a=dx^a/d\lambda$. Following Synge,[13] we can construct a null Frenet–Serret tetrad along the trajectory comprising two null vectors, the first of which is ξ^a, and two mutually orthogonal unit spacelike vectors, each of which is orthogonal to the null vectors. These vectors satisfy the null F–S equations,

$$\begin{bmatrix} \xi^{c'} \\ a^{c'} \\ \eta^{c'} \\ b^{c'} \end{bmatrix} = \begin{bmatrix} 0 & \kappa_1 & 0 & 0 \\ \kappa_2 & 0 & \kappa_1 & 0 \\ 0 & \kappa_2 & 0 & \kappa_3 \\ \kappa_3 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \xi^c \\ a^c \\ \eta^c \\ b^c \end{bmatrix}, \tag{30a}$$

(30b)

(30c)

(30d)

where $' \equiv \xi^a \nabla_a$ and $\xi^c \eta_c = 1 = -a^c a_c = -b^c b_c$, all other inner products between the vectors being zero. The scalar coefficients or curvatures are given by

$$\kappa_1 = k, \quad \kappa_2 = \tfrac{1}{2} k^{-3}(k'^2 + K), \quad \kappa_3 = k^{-5}\Delta, \tag{31}$$

where

$$k = (-\xi^{c\prime}\xi'_c)^{1/2}, \quad K = \xi^{c\prime\prime}\xi''_c \text{ and } \Delta = \eta^{abcd}\xi_a\xi'_b\xi''_c\xi'''_d.$$

Since ξ^a is an HK vector here, we can use Eq. (1) to write

$$\xi^{c\prime} = A^{cd}\xi_d + \phi\xi^c, \quad A_{cd} \equiv -\nabla_{[c}\xi_{d]}. \tag{32}$$

Obviously A^{cd} is a bivector. Furthermore, by making use of Eq. (7) we find that

$$A^{cd\prime} = 0. \tag{33}$$

The procedure now is similar to that used for the timelike curves. From Eqs. (30a) and (32) we have that $\kappa_1 a^c = A^{cd}\xi_d + \phi\xi^c$. By differentiating this and using equation (30a), it follows that

$$\kappa_1' a^c + \kappa_1 a^{c\prime} = \kappa_1 A^{cd} a_d + \kappa_1 \phi a^c. \tag{34}$$

We transvect Eq. (34) with a_c. Since $a^c a_c = -1$ and A^{cd} is antisymmetric, we have that

$$\kappa_1' = \kappa_1\phi \quad \text{and} \quad a^{c\prime} = A^{cd}a_d. \tag{35}$$

Equation (35) together with Eq. (30b) yield $\kappa_2\xi^c + \kappa_1\eta^c = A^{cd}a_d$. Again we repeat the above procedure and find that

$$\kappa_1' = \kappa_1\phi, \quad \kappa_2' = -\kappa_2\phi, \quad \kappa_3' = -\kappa_3\phi \tag{36a}$$

or

$$\kappa_1 = \kappa_{10}e^{\phi\lambda}, \quad \kappa_2 = \kappa_{20}e^{-\phi\lambda}, \quad \kappa_3 = \kappa_{30}e^{-\phi\lambda}, \tag{36b}$$

where the subscript "0" refers to the reference point $\lambda = 0$. Furthermore,

$$\begin{aligned} &\xi^{c\prime} = A^{cd}\xi_d + \phi\xi^c, \quad a^{c\prime} = A^{cd}a_d, \\ &\eta^{c\prime} = A^{cd}\eta_d - \phi\eta^c, \quad b^{c\prime} = A^{cd}b_d. \end{aligned} \tag{37}$$

We note the sign difference between κ_1 on the one hand and κ_2 and κ_3 on the other. In reference to this, it is interesting to take note of the following point made by Bonnor.[8] Unlike timelike curves that generally have three intrinsic scalars, nongeodesic null curves have only two curvatures, κ_2 and κ_3, that are arbitrary functions of the pseudo-arc (a particular parameter used by Bonnor). In flat spacetime he introduces a third curvature, κ_1, which has only two values, 0 or 1. The former corresponds to a straight line and the latter is introduced into his formalism to take account of a peculiar nonstraight curve, the null cubic, which has $\kappa_2 = \kappa_3 = 0$. We should not find it surprising, therefore, that we can distinguish between a nonessential curvature κ_1 and the essential curvatures κ_2 and κ_3. In fact with a suitable reparametrization we can also set $\kappa_1 = 1$. When $\phi = 0$, we have nongeodesic null Killing trajectories for which κ_1, κ_2, and κ_3 are constants of the motion. In flat spacetime these correspond to the null helices considered by Bonnor.

We obtain further relations by operating on ξ^b with the bievector identity $(A^4)^a{}_b - \bar{\alpha}(A^2)^a{}_b - \bar{\beta}^2\delta^a{}_b = 0$ where $\bar{\alpha} = -\tfrac{1}{2}A^{cd}A_{cd}$ and $\bar{\beta} = -\tfrac{1}{4}A^{cd}\hat{A}_{cd}$. By repeatedly applying Eqs. (36) and (37), we arrive at

$$\begin{aligned} 0 = &[\kappa_1^2(2\kappa_2^2 + \kappa_3^2) + 3\kappa_1\kappa_2\phi^2 - \bar{\alpha}\kappa_1\kappa_2 - \bar{\alpha}\phi^2 + \phi^4 - \bar{\beta}^2]\xi^c \\ &- [2\kappa_1^2\kappa_2\phi + \kappa_1\phi^3 - \kappa_1\phi\bar{\alpha}]a^c + [2\kappa_1^3\kappa_2 + \kappa_1^2\phi^2 - \kappa_1^2\bar{\alpha}]\eta^c. \end{aligned} \tag{38}$$

Transvecting Eq. (38) with either a_c or ξ_c leads to

$$0 = 2\kappa_1\kappa_2 + \phi^2 - \bar{\alpha}. \tag{39}$$

Again, transvecting Eq. (38) with η_c and making use of Eq. (39) leads to

$$\kappa_1^2\kappa_3^2 = \bar{\beta}^2. \tag{40}$$

From Eqs. (32) and (1) $\bar{\alpha}$ reduces to

$$\bar{\alpha} = 2\phi^2 - \tfrac{1}{2}\nabla^c\xi^d\nabla_c\xi_d, \tag{41}$$

[which is a renormalization of α; see Eq. (26)] from which

$$2\kappa_1\kappa_2 = \phi^2 - \tfrac{1}{2}\nabla^c\xi^d\nabla_c\xi_d. \tag{42}$$

From Eq. (36b) it follows that $\kappa_1\kappa_2$ and $\kappa_1\kappa_3$ are both constants and since ϕ is constant we have that $\nabla^c\xi^d\nabla_c\xi_d$ and $\nabla^c\xi^d(\nabla_c\xi_d)$ are constant along each trajectory.

Now we consider the rotation vector of this null congruence, i.e., $\bar{\omega}^a = \tfrac{1}{2}\eta^{abcd}\xi_b\nabla_c\xi_d$. With the help of Eq. (32) we can write this as

$$\bar{\omega}^c = -\hat{A}^{cd}\xi_d, \tag{43}$$

where $\hat{A}^{cd}$ is the dual of A^{cd}. Furthermore, the bivector identity[10] $(A^3)^{cd} - \bar{\alpha}A^{cd} - \bar{\beta}\hat{A}^{cd} = 0$ together with Eq. (43) yields

$$\bar{\beta}\bar{\omega}^c = \bar{\alpha}A^{cd}\xi_d - (A^3)^{cd}\xi_d. \tag{44}$$

Equations (36), (37), and (39) reduce this to $\bar{\beta}\bar{\omega}^c = -\kappa_1^2\kappa_3 b^c$. The norm of both sides of this equation together with Eq. (40) finally gives us

$$\bar{\omega}^c = \kappa_1 b^c, \quad \bar{\omega}^c\bar{\omega}_c = -\kappa_1^2, \tag{45}$$

where we have chosen the positive square root for $\bar{\omega}^c$.

We can now apply the foregoing to a homothetic stationary limit hypersurface defined by $\xi^c\xi_c = 0$. From Eq. (1) we see directly that the normal $n_c = \xi^d\nabla_c\xi_d$ is orthogonal to ξ^c, i.e., $\xi^c n_c = 0$. It follows that ξ^c lies in this hypersurface. We also note that ξ^c cannot be tangent to a null geodesic unless the hypersurface is also a null surface. For if we assume that ξ^c is tangent to a null geodesic, then we can write $\xi^{c\prime} = h\xi^c$ where h is a scalar function. Now the normal to the hypersurface n_c can be expressed, with the help of Eq. (1), as

$$n_c = 2\phi\xi_c - \xi'_c, \tag{46}$$

and in this case this reduces to $n_c = (2\phi - h)\xi_c$ or $n^c n_c = (2\phi - h)^2\xi^c\xi_c = 0$. Thus the homothetic stationary limit

surface is either a null hypersurface or else $2\phi = h$ in which case its normal is the zero vector! As an example, we can consider the stationary limit surface corresponding to the time-translational Killing vector ($\phi = 0$) of Kerr spacetime. There $n^a n_a \neq 0$ though $\xi^a \xi_a = 0$ and so these Killing trajectories are nongeodesic and null.

Finally, Eqs. (46) and (30a) yield

$$n_c = 2\phi\xi_c - \kappa_1 a_c, \quad n^c n_c = -\kappa_1^2. \tag{47}$$

We observe that Eqs. (45) and (47) can be combined as

$$\bar{\omega}^c \bar{\omega}_c - n^c n_c = 0. \tag{48}$$

This last result is simply Eq. (29) evaluated on the stationary limit surface. While our earlier derivation was based on a timelike formalism, our approach here made use of a null F—S process on the hypersurface itself. In any case, we see that if $\bar{\omega}^c \bar{\omega}_c \neq 0$ on the hypersurface, then it is not a null surface which in turn implies that it cannot be a horizon.

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[11]The negative root was first considered[3] in connection with the spacetime trajectories of charged particles in homogeneous electromagnetic fields. This was done to ensure the right-handedness of the spacelike triad $e_{(1)}$, $e_{(2)}$, and $e_{(3)}$. Since Killing trajectories bear a very strong resemblance to these world lines, the sign convention was retained.
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[13]Our choice of metric signature, -2, is different from Synge's.

The ionization T matrix

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The existence of the energy-shell limit of the "post" and "prior" forms of the half-off-shell T matrix is considered for N-particle scattering involving at most one charged fragment in the incoming channel. An approximate expression for the T matrix corresponding to the ionization of an uncharged fragment, consisting of two charged particles, by a charged particle is proposed.

I. INTRODUCTION

When there is more than one charged fragment in both the incoming and outgoing channels the usual expression for the half-off-shell T matrix must be "renormalized" before the on-energy-shell limit is performed.[1] These difficulties associated with the definition of the physical T matrix can be circumvented for scattering processes involving at most one charged fragment in either the incoming or outgoing channels. The particular case of scattering with at most one charged fragment in the incoming channel and more than one charged fragment in the outgoing channel is considered in Sec. III of this paper. The existence of the energy-shell limit of the "prior" form[2] of the half-off-shell T matrix is shown and a discussion of the breakdown of the "post" form of the half-off-shell T matrix is given.

In Sec. V of this paper we consider the problem of constructing the three particle ionization T matrix corresponding to an incoming channel with one charged fragment and an outgoing channel with three charged particles. In order to construct the ionization T matrix the three particle wavefunction corresponding to the free channel is required. In Sec. IV approximate three particle wavefunctions corresponding to the free channel are proposed. The justification of this approximation is based on the time-dependent theory for Coulomb scattering and is independent of the existence of integral equations for the physical wavefunctions.

The approximate wavefunctions proposed in Sec. IV are applied in Sec. V to obtain an approximate expression for the ionization T matrix. A discussion of the relationship of this approximation to the usual Born approximation for the ionization T matrix[3,4] is given.

II. PRELIMINARIES

In this paper we assume the scattering system consists of N distinguishable spinless particles interacting via two-body Coulomb-like potentials. We assume the Hamiltonian $\tilde{H}$ has the form

$$\tilde{H}=\tilde{H}_0+\sum_{i<j}V_{ij},\quad \tilde{H}_0=\sum_{i=1}^{N}(-2\mu_i)^{-1}\nabla_i^2,$$
$$V_{ij}(\mathbf{x})=e^2V_{ij}^c(\mathbf{x})+V_{ij}^s(\mathbf{x}),\quad V_{ij}^c(\mathbf{x})=Z_iZ_j|\mathbf{x}|^{-1}, \tag{2.1}$$

where μ_i and Z_ie are respectively the mass and charge of particle i and $V_{ij}^s\in L^2(R^3)+L^p(R^3)$, $2<p<3$, $1\le i<j\le N$.

The "modified" or "renormalized" wave operators for N-particle Coulomb scattering are defined as follows,[5,6]

$$\tilde{\Omega}_{\pm}^{(\gamma)}=\operatorname*{s-lim}_{t\to\pm\infty}\exp(i\tilde{H}t)\exp[-i\tilde{H}_\gamma t-iG^{(\gamma)}(t)]\tilde{P}^{(\gamma)}, \tag{2.2}$$

where $\tilde{H}_\gamma$ is the γ-channel Hamiltonian, $\tilde{P}^{(\gamma)}$ is the projection onto $\tilde{H}^{(\gamma)}$, the γ-channel subspace, and $G^{(\gamma)}(t)=\sum_{j<k}G_{jk}^{(\gamma)}(t)$, where for $1\le j<k\le n_\gamma$

$$G_{jk}^{(\gamma)}(t)=\epsilon(t)\frac{M_jM_ke_je_k}{|\mathbf{P}_{jk}|}\log\left(\frac{2|t+\epsilon(t)|\mathbf{P}_{jk}|^2}{M_jM_k(M_j+M_k)}\right)$$

$$\epsilon(t)=\begin{cases}1, & t>0,\\ -1, & t<0,\end{cases} \tag{2.3}$$

where M_j, e_j, and $\mathbf{P}_j$ denote respectively the total mass, total charge, and the center-of-mass momenta of the jth fragment and $\mathbf{P}_{jk}=M_k\mathbf{P}_j-M_j\mathbf{P}_k$, $1\le j<k\le n_\gamma$, where n_γ denotes the number of fragments making up the channel γ. The existence of the renormalized wave operators have been shown for a general class of Coulomb-like potentials.[5,6] It is important to note that when there is at most one charged fragment in the channel γ then $G^{(\gamma)}(t)=0$ and the renormalized wave operators reduce to the wave operators of short-range potential scattering which we denote by $\tilde{W}_{\pm}^{(\gamma)}$.

When deriving time-independent results it is convenient to separate off the total center-of-mass motion of the N-particle system. We denote the Hamiltonian corresponding to (2.1) after the total center-of-mass kinetic energy operator has been separated off by $H=H_0+\sum_{i<j}V_{ij}$. The explicit form of H depends on the choice of "internal" position variables which will be denoted collectively by $x\in R^{3(N-1)}$. The Hilbert space $\tilde{H}=L^2(R^{3N})$ can be written as $\tilde{H}=L^2(R^3)\otimes H$, $H=L^2(R^{3(N-1)})$ and the γ-channel subspace takes the form $\tilde{H}^{(\gamma)}=L^2(R^3)\otimes H^{(\gamma)}$. Furthermore, $\tilde{\Omega}_{\pm}^{(\gamma)}=\Pi\otimes\Omega_{\pm}^{(\gamma)}$ and $\tilde{W}_{\pm}^{(\gamma)}=\Pi\otimes W_{\pm}^{(\gamma)}$ where $\Omega_{\pm}^{(\gamma)}$ and $W_{\pm}^{(\gamma)}$ act in H.

III. THE N-PARTICLE T MATRIX

The convergence of the prior form of the half-off-shell T matrix to the on-energy-shell T matrix is shown for scattering involving at most one charged fragment in the incoming channel and more than one charged fragment in the outgoing channel. We first give a short account of the prior and post forms of the half-off-shell T matrix for short-range potential scattering.

For short-range potential scattering the T operator $T_{\alpha\beta}$ corresponding to an initial two fragment channel α and final channel β is defined in terms of the wave operators, $W_{\pm}^{(\gamma)}$, by $T_{\alpha\beta}=-(2\pi i)^{-1}(\delta_{\alpha\beta}P^{(\beta)}-W_+^{(\beta)*}W_-^{(\alpha)})$. Due to the orthogonality of the ranges of the wave operators for different channels we can rewrite $T_{\alpha\beta}$ as follows

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$$T_{\alpha\beta} = -(2\pi i)^{-1} W_+^{(\beta)*}(W_+^{(\alpha)} - W_-^{(\alpha)})$$
$$= -(2\pi i)^{-1}(W_-^{(\beta)*} - W_+^{(\beta)*}) W_-^{(\alpha)}. \quad (3.1)$$

The wave operators have the following Riemann–Stieltjes integral representations,[7-9]

$$W_\pm^{(\gamma)} = \operatorname{s-lim}_{\epsilon\to+0} \int_{-\infty}^{+\infty} \frac{\pm i\epsilon}{H - \lambda \pm i\epsilon} d_\lambda E_\lambda^{H_\gamma} P^{(\gamma)}. \quad (3.2)$$

Applying (3.2) and the intertwining properties[9] to the first equality in (3.1) leads to the "prior" form of the T operator

$$T_{\alpha\beta}\psi = \operatorname{s-lim}_{\epsilon\to+0}(-\pi)^{-1} \int_{-\infty}^{+\infty} \frac{\epsilon}{(H_\beta - \lambda)^2 + \epsilon^2}$$
$$\times W_+^{(\beta)*}(H - \lambda)\, d_\lambda E_\lambda^{H_\alpha} P^{(\alpha)}\psi, \quad (3.3)$$

where $\psi \in \mathcal{D}(H_\alpha)$. A similar argument applied to the second equality in (3.1) leads to the "post" form of the T operator,

$$T_{\alpha\beta} = \operatorname{w-lim}_{\epsilon\to+0}(-\pi)^{-1} P^{(\beta)} \int_{-\infty}^{+\infty} d_\lambda E_\lambda^{H_\beta} (H - \lambda) W_-^{(\alpha)} \frac{\epsilon}{(H_\alpha - \lambda)^2 + \epsilon^2}. \quad (3.4)$$

By a lengthy but straightforward argument one can relate the prior and post forms of the T operator to the usual prior and post forms of the half-off-shell T matrix. The derivation of this relationship is outlined below for scattering involving Coulomb-like potentials and will not be given in the short-range case.

We now consider a two fragment incoming channel α consisting of at most one charged fragment and an outgoing channel β consisting of more than one charged fragment. The T operator is given by $T_{\alpha\beta} = (2\pi i)^{-1}\Omega_+^{(\beta)*} W_-^{(\alpha)}$. A similar argument as applied in the short-range case shows that the prior form of the T operator is valid [Eq. (3.11), Ref. 10 with $F_\epsilon^{(\alpha)} = 1$], i.e., $T_{\alpha\beta}$ has the following stationary representation

$$T_{\alpha\beta}\psi = \operatorname{s-lim}_{\epsilon\to+0}(-\pi)^{-1} \int_{-\infty}^{+\infty} \frac{\epsilon}{(H_\beta - \lambda)^2 + \epsilon^2} \Omega_+^{(\beta)*} V^{(\alpha)} d_\lambda E_\lambda^{H_\alpha} P^{(\alpha)}\psi, \quad (3.5)$$

where $\psi \in \mathcal{D}(H_\alpha)$ and $V^{(\alpha)} = H - H_\alpha$. The post form of the T operator is not valid since the renormalized wave operators $\Omega_\pm^{(\beta)}$ do not have the stationary representations (3.2), however a "renormalized" post form of the T operator is valid [Eq. (3.10), Ref. 10 with $\Omega_-^{(\alpha)} = W_-^{(\alpha)}$].

It is not difficult to show (see Sec. III, Ref. 1) that (3.5) can be written as follows,

$$T_{\alpha\beta}\psi = \operatorname{s-lim}_{\epsilon\to+0} \operatorname{s-lim}_{R\to\infty}(-\pi)^{-1} \int_{-\infty}^{+\infty} \frac{\epsilon}{(H_\beta - \lambda)^2 + \epsilon^2} \quad (3.6)$$
$$\times \Omega_+^{(\beta)*} g_R V^{(\alpha)} d_\lambda E_\lambda^{H_\alpha} P^{(\alpha)}\psi,$$

where g_R is any cutoff function which satisfies: $|g_R(\mathbf{x})| \le C$ for all $\mathbf{x} \in R^3$ where C is a constant, $g_R V^{(\alpha)} \eta_1\eta_2 \in L^1[R^{3(N-1)}]$ for each $0 < R < \infty$ where η_1 and η_2 are the bound state wavefunctions making up the channel α and $\lim_{R\to\infty} g_R(\mathbf{x}) = 1$ for all $\mathbf{x} \in R^3$.

In order to relate (3.6) to the usual expression for the prior form of the half-off-shell T matrix we assume the β-channel wavefunction $\phi_-^{(\beta)}(x, p_\beta)$, where p_β denotes a set of relative momenta variables of the n_β fragments, satisfies

$$(\Omega_+^{(\beta)}\psi)(x) = \text{l. i. m.} \int dp_\beta \phi_-^{(\beta)}(x, p_\beta)\hat{\psi}_1(p_\beta) \quad (3.7)$$

for $\psi = \psi_1 \Pi_{l=1}^{n_\beta} \xi_l \in H^{(\beta)}$ where ξ_l is the bound state wavefunction of the lth fragment, $1 \le l \le n_\beta$, and $\hat{\psi}_1$ is the Fourier transform of ψ_1. In addition we assume that $\phi_-^{(\beta)}(x, p_\beta)$ satisfies for almost all $x \in R^{3(N-1)}$

$$\int dp_\beta |\phi_-^{(\beta)}(x, p_\beta)\hat{\psi}_1(p_\beta)| \le C, \quad (3.8)$$

where C is a finite constant for each $\psi_1 \in \mathcal{J}$ with $\mathcal{J}$ a dense subset of $S(R^{3(n_\beta - 1)})$. Under these assumptions we obtain (see Sec. 2 VII, of Ref. 1) the following relationship between (3.6) and the prior form of the half-off-shell T matrix

$$\langle\psi|\, T_{\alpha\beta}\phi\rangle = \lim_{\epsilon\to+0} \lim_{R\to\infty}(-\pi)^{-1} \int dp_\beta dp_\alpha \overline{\hat{\psi}_1(p_\beta)}\hat{\phi}_1(p_\alpha)$$
$$\times (p_\beta|\, T_{\alpha\beta}(R)\,|p_\alpha) \frac{\epsilon}{(E^{(\alpha)} - E^{(\beta)})^2 + \epsilon^2}, \quad (3.9)$$

where $\psi = \psi_1 \Pi_{l=1}^{n_\beta} \xi_l \in H^{(\beta)}$, $\psi_1 \in \mathcal{J}$, $\phi_1\eta_1\eta_2$, $\phi_1 \in S(R^3)$, and

$$(p_\beta|\, T_{\alpha\beta}(R)\,|p_\alpha) = \int dx\, \overline{\phi_-^{(\beta)}(x, p_\beta)}(g_R V^{(\alpha)})(x)\phi^{(\alpha)}(x, p_\alpha) \quad (3.10)$$

with $H_\gamma \phi^{(\gamma)}(x, p_\gamma) = E^{(\gamma)}\phi^{(\gamma)}(x, p_\gamma)$.

An application of the nuclear theorem[11,12] yields the existence of the physical on-energy-shell T matrix, denoted $(p_\beta|\, T_{\alpha\beta}\,|p_\alpha)_{E^{(\beta)} = E^{(\alpha)}}$, as a tempered distribution, i.e.,

$$\langle\psi|\, T_{\alpha\beta}\phi\rangle = \int dp_\beta dp_\alpha \overline{\hat{\psi}_1(p_\beta)}\hat{\phi}_1(p_\alpha)(p_\beta|\, T_{\alpha\beta}\,|p_\alpha)_{E^{(\beta)} = E^{(\alpha)}} \quad (3.11)$$

for $\psi_1 \in S(R^{3(n_\beta - 1)})$, $\phi_1 \in S(R^3)$.

We conclude from (3.9) and (3.11) that for scattering corresponding to an initial channel with at most one charged fragment and final channel involving more than one charged fragment the usual prior form of the half-off-shell T matrix has a well defined energy-shell limit. The post form of the half-off-shell T matrix must be "renormalized" before the energy-shell limit is performed (see Theorem 7.2, Ref. 1).

IV. APPROXIMATE THREE PARTICLE WAVEFUNCTIONS

In order to calculate the three particle ionization T matrix via the prior form of the half-off-shell T matrix the three particle wavefunction $\phi_-(x, p)$ [$\phi_-^{(\beta)}(x, p_\beta)$ with $\beta = 0$] is required. Let $x = \{\mathbf{x}_k, \mathbf{x}_{ij}\}$, $1 \le i < j \le 3$, $k \ne i, j$, where $\mathbf{x}_k$ and $\mathbf{x}_{ij}$ are defined in terms of the position coordinates $\{\mathbf{y}_i, \mathbf{y}_j, \mathbf{y}_k\}$ of the three particles as follows,

$$\mathbf{x}_{ij} = \mathbf{y}_j - \mathbf{y}_i,$$
$$\mathbf{x}_k = \mathbf{y}_k - (\mu_i + \mu_j)^{-1}(\mu_i \mathbf{y}_i + \mu_j \mathbf{y}_j).$$

Furthermore let $\phi_\pm^{ij}(x, p)$, $1 \le i < j \le 3$ be defined in terms of the coordinates $x = \{\mathbf{x}_{ij}, \mathbf{x}_k\}$ and $p = \{\mathbf{p}_{ij}, \mathbf{p}_k\}$ by

$$\phi_\pm^{ij}(x, p) = \phi(\mathbf{x}_k, \mathbf{p}_k)\phi_\pm(\mathbf{x}_{ij}, \mathbf{p}_{ij}), \quad k \ne i, j,$$

where $\phi(\mathbf{x}_k, \mathbf{p}_k)$ denotes the two particle free wavefunction and $\phi_\pm(\mathbf{x}_{ij}, \mathbf{p}_{ij})$ denote the two particle Coulomb wavefunctions. In this section we propose that the three

particle wavefunctions $\phi_\pm(x,p)$ can be approximated as follows,

$$\phi_\pm(x,p) \approx \phi(x,p) - \sum_{i<j}[\phi(x,p) - \phi_\pm^{ij}(x,p)] \tag{4.1}$$

as $e \to 0$ where $\phi(x,p)$ denotes the three particle free wavefunction.

The approximate wavefunctions (4.1) have the form of the nonhomogeneous term appearing in the Faddeev equations for the three particle wavefunctions. One cannot however justify the approximation (4.1) via the Faddeev equations since these equations are not valid for the Coulomb wavefunctions $\phi_\pm(x,p)$.

The approximation (4.1) can be obtained from a formal "renormalized" perturbation expansion for the three particle wavefunctions $\phi_\pm(x,p)$. This expansion can be defined in an analogous fashion as in the two particle case,[13] however a justification of this formal perturbation expansion is lacking in the three particle case.

The motivation given in this paper for the approximation (4.1) is based on the following result for the renormalized wave operators $\Omega_\pm^{(0)}$

$$\lim_{\epsilon\to 0}\left\langle \phi \,|\, e^{-\beta}\left[\Omega_\pm^{(0)} - \Pi + \sum_{i<j}(\Pi - \Omega_\pm^{ij})\right]\psi\right\rangle = 0, \quad \beta < 4 \tag{4.2}$$

valid for $\phi,\ \psi \in S_c(R^6)$ where S_c is a dense subset of H and for $1 \le i < j \le 3$

$$\Omega_\pm^{ij} = \operatorname*{s-lim}_{t\to\pm\infty} \exp(iH_{ij}t)\exp[-iH_0t - iG_{ij}(t)] \tag{4.3}$$

with $H_{ij} = H_0 + V_{ij}$. Assuming that the expansion (3.7) is valid for $\beta = 0$ (with a similar expansion for $\Omega_-^{(0)}$) (4.2) can be rewritten as follows,

$$\lim_{\epsilon\to 0}\int dx\, \overline{\phi(x)} \int dp\, \hat{\psi}(p)\, e^{-\beta}\{\phi_\mp(x,p) - \phi(x,p) + \sum_{i<j}[\phi(x,p) - \phi_\mp^{ij}(x,p)]\} = 0, \quad \beta < 4 \tag{4.4}$$

for each $\phi, \psi \in S_c(R^6)$. The result (4.4) is a precise statement of the approximation (4.1).

In order to verify (4.2) it is sufficient to show

$$\lim_{\epsilon\to 0}\left\langle \phi \,|\, e^{-\beta}\left[\tilde{\Omega}_\pm^{(0)} - \Pi + \sum_{i<j}(\Pi - \tilde{\Omega}_\pm^{ij})\right]\psi\right\rangle = 0, \quad \beta < 4 \tag{4.5}$$

for $\phi, \psi \in \tilde{S}_c(R^9)$ where $\tilde{S}_c$ denotes the set of Schwartz functions $f(x)$ whose Fourier transform $\hat{f}(p)$ vanishes in a neighborhood of $\mu_i \mathbf{p}_j = \mu_j \mathbf{p}_i$, $1 \le i < j \le 3$.

We now consider the operators $\hat{\Omega}_\pm = \tilde{\Omega}_\pm^{(0)} - \Pi + \sum_{i<j}(\Pi - \tilde{\Omega}_\pm^{ij})$. For each $\psi \in \tilde{S}_c$ the operators $\tilde{\Omega}_\pm^{(0)}$ and $\tilde{\Omega}_\pm^{ij}$, $1 \le i < j \le 3$ satisfy

$$(\tilde{\Omega}_\pm^{(0)} - \Pi)\psi = e^2 \sum_{i<j} i\int_0^{\pm\infty} dt \exp(i\tilde{H}t)\left[V_{ij}^c - \frac{d\hat{G}_{ij}(t)}{dt}\right] \times \exp(-i\tilde{H}_0 t - iG^{(0)}(t))\,\psi,$$

$$(\tilde{\Omega}_\pm^{ij} - \Pi)\psi = e^2 i\int_0^{\pm\infty} dt \exp(i\tilde{H}_{ij}t)\left[V_{ij}^c - \frac{d\hat{G}_{ij}(t)}{dt}\right] \times \exp(-i\tilde{H}_0 t - iG_{ij}(t))\,\psi,$$

where $G_{ij} = e^2\hat{G}_{ij}$, $1 \le i < j \le 3$. Thus for $\psi \in \tilde{S}_c$ we have

$$\begin{aligned}\langle \phi \,|\, \tilde{\Omega}_\pm \psi\rangle &= e^2 \sum_{i<j} i\int_0^{\pm\infty} dt \langle \phi \,|\, \exp(i\tilde{H}t) \times \left[V_{ij}^c - \frac{d\hat{G}_{ij}(t)}{dt}\right]\exp(-i\tilde{H}_0 t) \\ &\times [\exp(-iG^{(0)}(t)) - \exp(-iG_{ij}(t))]\,\psi\rangle \\ &+ e^2 \sum_{i<j} i\int_0^{\pm\infty} dt \langle \phi \,|\, [\exp(i\tilde{H}t) - \exp(i\tilde{H}_{ij}t)] \\ &\times \left[V_{ij}^c - \frac{d\hat{G}_{ij}(t)}{dt}\right]\exp(-i\tilde{H}_0 t - iG_{ij}(t))\,\psi\rangle. \end{aligned} \tag{4.6}$$

In order to verify (4.5) we require the following technical lemma.

Lemma: For each constant $0 < R < \infty$ and for each $\psi \in \tilde{S}_c$ there exist constants D_1, D_2 and D_3 which are independent of e for $|e| < R$ such that

(a) $$\sum_{i<j}(\pm)\int_0^{\pm\infty} dt \left\| \left[V_{ij}^c - \frac{d\hat{G}_{ij}(t)}{dt}\right]\exp(-i\tilde{H}_0 t) \times [\exp(-iG^{(0)}(t)) - \exp(-iG_{ij}(t))]\,\psi\right\| \le |e|^2 D_1. \tag{4.7}$$

(b) For $1 \le i < j \le 3$

$$\left\| \left[V_{ij}^c - \frac{dG_{ij}(t)}{dt}\right]\exp[-i\tilde{H}_0 t - iG_{ij}(t)]\,\psi\right\| \le D_2(1 + |t|)^{-3/2}[\log(1 + |t|)]^\mu, \tag{4.8}$$

where μ is a positive constant.

(c) For $1 \le i < j \le 3$

$$\| V_{kl}^c \exp(-i\tilde{H}_{ij}t)\,\psi\| \le D_3(1 + |t|)^{-1}, \tag{4.9}$$

where $1 \le k < l \le 3$, $k \ne i, j$ or $l \ne i, j$, $\tilde{H}_{ij} = \tilde{H}_0 + e^2 V_{ij}^c$.

Parts (a) and (b) of the above lemma can be verified by a slight modification of Dollard's proof of the existence of the renormalized wave operators.[6] Part (c) of the above lemma is verified in the Appendix.

The above lemma together with (4.6) yields

$$|\langle \phi \,|\, \hat{\Omega}_+ \psi\rangle| \le D|e|^4$$

for $\phi, \psi \in \tilde{S}_c$ where D is a constant independent of $|e| < R$ which verifies (4.5).

V. AN APPROXIMATE IONIZATION T MATRIX

The three particle ionization T matrix denoted by $(p \,|\, T_I \,|\, p_\alpha)_{E^{(\alpha)}=E^{(0)}}$ is given by

$$(p \,|\, T_I \,|\, p_\alpha)_{E^{(\alpha)}=E^{(0)}} = \int dx\, \overline{\phi_-(x,p)}\, V^{(\alpha)}(x)\phi^{(\alpha)}(x,p_\alpha)\big|_{E^{(\alpha)}=E^{(0)}}, \tag{5.1}$$

where $\phi_-(x,p)$ denotes the three particle wavefunction corresponding to the free channel. We must emphasize that (5.1) is a formal expression for the ionization T matrix which is rigorously defined in terms of the limits $R \to \infty$ and $\epsilon \to +0$ of the prior form of the half-off-shell T matrix as in (3.9).

Applying the approximation (4.1) for $\phi_-(x,p)$ we obtain the following approximate expression for the ionization T matrix,

$$(p|T_I|p_\alpha)_{E^{(\alpha)}=E^{(0)}} \approx \{\int dx\, \overline{\phi(x,p)}\, V^{(\alpha)}(x)\phi^{(\alpha)}(x,p_\alpha) - \sum_{i<j}\int dx[\overline{\phi(x,p)} - \overline{\phi_-^{ij}(x,p)}]\, V^{(\alpha)}(x)\phi^{(\alpha)}(x,p_\alpha)\}|_{E^{(\alpha)}=E^{(0)}}. \tag{5.2}$$

In order to compare (5.2) with the usual Born approximation we assume the uncharged fragment of the channel α consists of particles 1 and 2 and the charged fragment corresponds to particle 3. The usual Born approximation for the ionization T matrix (5.1) takes the form[3,4]

$$(p|T_B|p_\alpha)_{E^{(\alpha)}=E^{(0)}} = \int dx\, \overline{\phi_-^{12}(x,p)}\, V^{(\alpha)}(x)\phi^{(\alpha)}(x,p_\alpha)|_{E^{(\alpha)}=E^{(0)}}. \tag{5.3}$$

One difficulty with the Born approximation is the lack of symmetry in the approximate final channel wavefunction. The approximation (5.2) does not suffer this problem since the approximate final channel wavefunction (4.1) does not distinguish between any of the three particles in the final channel.

The approximation (5.2) formally reduces to the Born approximation when particle 3 has a high relative momentum with respect to particles 1 and 2. Thus for scattering in which particle 3 has a much greater energy than the outgoing particles 1 and 2 we expect the Born approximation (5.3) to be valid. When all three final particles have high comparable energies we expect the approximation (5.2) to be valid.

APPENDIX

In order to verify (4.9) we assume $i=k=1$, $j=2$ and $l>0$ (the various other cases can be verified by an analogous argument) and rewrite $\tilde{H}_{12}$ and V_{13}^c in terms of the coordinates $\mathbf{x}=(\mu_1\mathbf{y}_1+\mu_2\mathbf{y}_2)/(\mu_1+\mu_2)$, $\mathbf{x}_{12}=\mathbf{y}_2-\mathbf{y}_1$, and $\mathbf{x}_3=\mathbf{y}_3$ as follows:

$$\begin{aligned}\tilde{H}_{12} &= -(2\mu)^{-1}\nabla_{\mathbf{x}_{12}}^2 - [2(\mu_1+\mu_2)]^{-1}\nabla_{\mathbf{x}}^2 - (2\mu_3)^{-1}\nabla_{\mathbf{x}_3}^2 + V_{12}^c(\mathbf{x}_{12})\\ &= H_{12}^I + H_0^I,\\ H_0^I &= -[2(\mu_1+\mu_2)]^{-1}\nabla_{\mathbf{x}}^2 - (2\mu_3)^{-1}\nabla_{\mathbf{x}_3}^2,\end{aligned}$$

and

$$V_{13}^c = Z_1Z_3|\mathbf{x}-\frac{\mu}{\mu_1}\mathbf{x}_{12}-\mathbf{x}_3|^{-1},$$

where

$$\mu=\frac{\mu_1\mu_2}{\mu_1+\mu_2}.$$

The right side of (4.9) satisfies the following inequality,

$$\|V_{13}^c\exp(-i\tilde{H}_{12}t)\psi\| \le \|[V_{13}^c - V^c]\exp(-i\tilde{H}_{12}t)\psi\| + \|V^c\exp(-i\tilde{H}_{12}t)\psi\|, \tag{A1}$$

where $V^c = Z_1Z_3|\mathbf{x}-\mathbf{x}_3|^{-1}$. A slight modification of the argument used to prove the existence of the renormalized wave operators[5,6] yields the following estimate for the last term in (A1)

$$\|V^c\exp(-i\tilde{H}_{12}t)\psi\| = \|V^c\exp(-iH_0^It)\psi\| \le C(1+|t|)^{-1},$$

where the constant C depends on $\psi\in\tilde{S}_c$. Thus in order to complete the proof of (4.9) we must show

$$\|(V_{13}^c - V^c)\exp(-i\tilde{H}_{12}t)\psi\| \le C'(1+t)^{-1}, \tag{A2}$$

where C' is a constant which depends on $\psi\in\tilde{S}_c$.

The right side of (A2) satisfies the following inequality,

$$\begin{aligned}&\|(V_{13}^c - V^c)\exp(-i\tilde{H}_{12}t)\psi\|\\ &\le \frac{\mu Z_1Z_3}{\mu_1}\left(\int d\mathbf{x}\,d\mathbf{x}_{12}\,d\mathbf{x}_3 \frac{|\mathbf{x}_{12}|^2}{|\mathbf{x}-\mathbf{x}_3|^2|\mathbf{x}-(\mu/\mu_1)\mathbf{x}_{12}-\mathbf{x}_3|^2} \times|\{\exp[-iH_0^I(t+1)-iH_{12}^It]\tilde{\psi}\}(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2\right)^{1/2},\end{aligned} \tag{A3}$$

where

$$\tilde{\psi}(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3) = [\exp(iH_0^I)\psi](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3).$$

The standard estimate

$$\begin{aligned}&[\exp[i(2\mu_3)^{-1}\nabla_{\mathbf{x}_3}^2(t+1)](\exp\{i[2(\mu_1+\mu_2)]^{-1}\\ &\times\nabla_{\mathbf{x}}^2(t+1)-iH_{12}^It\}\tilde{\psi})](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)\\ &=\left(\frac{\mu_3}{2\pi i(t+1)}\right)^{3/2}\int d\mathbf{y}_3\exp\left(\frac{i\mu_3}{2(t+1)}(\mathbf{x}_3-\mathbf{y}_3)^2\right)\\ &\times(\exp\{i[2(\mu_1+\mu_2)]^{-1}\nabla_{\mathbf{x}}^2(t+1)-iH_{12}^It\}\tilde{\psi})(\mathbf{x},\mathbf{x}_{12},\mathbf{y}_3)\end{aligned}$$

together with (A3) yields the following bound,

$$\begin{aligned}&\|(V_{13}^c - V^c)\exp(-i\tilde{H}_{12}t)\psi\|\\ &\le C_1(1+t)^{-3/2}\{\int d\mathbf{x}\,d\mathbf{x}_{12}|\mathbf{x}_{12}|[\int d\mathbf{y}_3|(\exp\{i[2(\mu_1+\mu_2)]^{-1}\\ &\times\nabla_{\mathbf{x}}^2(t+1)-iH_{12}^It\}\tilde{\psi})(\mathbf{x},\mathbf{x}_{12},\mathbf{y}_3)|^2]\}^{1/2}\\ &\le C_2(1+t)^{-3/2}[\int d\mathbf{x}\,d\mathbf{x}_{12}\,d\mathbf{x}_3|\mathbf{x}_{12}|\\ &\times|(\exp\{i[2(\mu_1+\mu_2)]^{-1}\nabla_{\mathbf{x}}^2(t+1)-iH_{12}^It\}\phi)(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2]^{1/2}\end{aligned}$$

where C_1 and C_2 are constants and $\phi(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3) = (1+|\mathbf{x}_3|^2)^n\tilde{\psi}(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)$ with $n\ge 2$. Thus for $\psi\in\tilde{S}_c$ we have

$$\begin{aligned}&\|(V_{13}^c - V^c)\exp(-i\tilde{H}_{12}t)\psi\|\\ &\le C_2(1+t)^{-3/2}\|\phi\|^{1/2}\{\int d\mathbf{x}\,d\mathbf{x}_{12}\,d\mathbf{x}_3|\mathbf{x}_{12}|^2\\ &\times|[\exp(-iH_{12}^It)\phi](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2\}^{1/4}.\end{aligned} \tag{A4}$$

Let $\mathbf{x}_{12}=(x_1,x_2,x_3)$. Theorem 5 of Ref. 14 with $n=1$ provides the following estimate,

$$\begin{aligned}&\{\int d\mathbf{x}_{12}|\mathbf{x}_{12}|^2|[\exp(-iH_{12}^It)\phi](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2\}^{1/2}\\ &\le\sum_{i=1}^3\{\int d\mathbf{x}_{12}|x_i|^2|[\exp(-iH_{12}^It)\phi](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2\}^{1/2}\\ &\le C_3(1+|t|)\left\{\sum_{i=1}^3[\int d\mathbf{x}_{12}|x_i|^2|\phi(\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2]^{1/2} + [\int d\mathbf{x}_{12}|[H_{12}^I\phi](\mathbf{x},\mathbf{x}_{12},\mathbf{x}_3)|^2]^{1/2}\right\}.\end{aligned} \tag{A5}$$

The inequality (A4) together with (A5) verifies (A2).

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An angle-dependent lower bound on the solution of the elastic unitarity integral and a new uniqueness condition resulting from it

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Through an iteration process we construct, from the angle-dependent upper bound to the unitarity integral, an angle-dependent lower bound and use this result to derive a uniqueness condition on the solution of the integral equation.

In a recent paper[1] we gave an angle-independent lower bound on the phase $[\sin\alpha(z)]$ of the scattering amplitude defined by the integral equation

$$\sin\alpha(z)=\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}\frac{|f(x)|\,|f(y)|}{|f(z)|}\times\cos[\alpha(x)-\alpha(y)]\,\frac{\Theta(K)}{K^{1/2}}\,dx\,dy, \tag{1}$$

where $|f(z)|$ is the modulus of the amplitude assumed to be known at all angles from a knowledge of the differential cross section. $\Theta(K)$ is the step function and $K=1-x^2-y^2-z^2+2xyz$. q is the center-of-mass wavenumber.

We define

$$\sin\mu(z)=\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}\frac{|f(x)|\,|f(y)|}{|f(z)|}\,\frac{\Theta(K)}{K^{1/2}}\,dx\,dy. \tag{2}$$

We call the supremum of $\sin\mu(z)$ in the interval $-1\leq z\leq+1$ "$\sin\mu$" and assume that $\sin\mu<1$. Its infinum will be called "$\sin\nu$." In the following discussion we shall use the notation $\mu(>\frac{x}{y})$, which will mean the larger of the values of μ at x or y. Similarly $\gamma(<\frac{x}{y})$ will mean the smaller of $\gamma(x)$ or $\gamma(y)$. We can now write

$$\sin\alpha(z)\geq\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}\frac{|f(x)|\,|f(y)|}{|f(z)|}\times\cos[\mu(>\tfrac{x}{y})-0]\,\frac{\Theta(K)}{K^{1/2}}\,dx\,dy\equiv\sin\gamma_1(z), \tag{3}$$

since $[\mu(>\frac{x}{y})-0]$ majorizes $[\alpha(x)-\alpha(y)]$, thus minimizing $\cos[\alpha(x)-\alpha(y)]$. The domain of $\alpha(z)$ is between 0 and $\pi/2$ (see the references given in Ref. 1). With $\gamma_1(z)\leq\alpha(z)$ we repeat the process[2]:

$$\sin\alpha(z)\geq\frac{q}{2}\int_{-1}^{+1}\int_{-1}^{+1}\frac{|f(x)|\,|f(y)|}{|f(z)}\times\cos[\mu(>\tfrac{x}{y})-\gamma_1(<\tfrac{x}{y})]\,\frac{\Theta(K)}{K^{1/2}}dx\,dy\equiv\sin\gamma_2(z)\geq\sin\gamma_1(z). \tag{4}$$

Continuing the iteration, we improve on $\sin\gamma_1(z)$ and call the limit $\sin\gamma(z)$

$$\lim_{i\to\infty}\sin\gamma_i(z)=\sin\gamma(z). \tag{5}$$

Thus we have

$$\sin\alpha(z)\geq\sin\gamma(z). \tag{6}$$

Unlike Ref. 1 where the value of the angle-independent lower bound $\sin\theta_{\min}$ could be expressed in terms of the supremum $\sin\mu$ and infinum $\sin\nu$ of the integral (2), $\sin\gamma(z)$ can only be found if $|f(z)|$ is explicitly known. The integrals of type (3) and (4) must be evaluated numerically.

In Ref. 1 we have used the angle-independent lower bound $\sin\theta_{\min}$ of $\sin\alpha(z)$ to extend the uniqueness domain for the solutions of the unitarity integral. This domain could be expressed in terms of the value of ν for a given μ. Similarly the angle-dependent lower bound $\sin\gamma(z)$ of $\sin\alpha(z)$ will be used to improve the uniqueness domain. The basic relation here is[3]

$$\begin{aligned}\mathrm{Im}f(z)-\mathrm{Im}g(z)&=\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}[\mathrm{Im}f(x)-\mathrm{Im}g(x)]\\&\times\left[\frac{\mathrm{Im}f(y)+\mathrm{Im}g(y)}{\mathrm{Re}f(y)+\mathrm{Re}g(y)}-\frac{\mathrm{Im}f(x)+\mathrm{Im}g(x)}{\mathrm{Re}f(x)+\mathrm{Re}g(x)}\right]\\&\times[\mathrm{Re}f(y)+\mathrm{Re}g(y)]\frac{\Theta(K)}{K^{1/2}}dx\,dy,\end{aligned} \tag{7}$$

where $f(z)$ and $g(z)$ are assumed to be two different solutions of the unitarity equation with equal moduli but different phases.

This relation can be written as

$$\begin{aligned}&|\mathrm{Im}f(z)-\mathrm{Im}g(z)|\\&\leq\max|\mathrm{Im}f-\mathrm{Im}g|\,\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}[\tan\mu(y)-\tan\gamma(x)]\\&\times[\mathrm{Re}f(y)+\mathrm{Re}g(y)]\frac{\Theta(K)}{K^{1/2}}\,dx\,dy.\end{aligned} \tag{8}$$

In the case of the angle-independent bounds, we were able to take the bracket with the tan terms outside the integral and the integrals of the real parts of the amplitudes gave us real parts of the s waves, which were bounded by $\frac{1}{2}$. Here we can no longer do this because of the angle-dependent factor multiplying the real parts of the amplitudes. We therefore majorize the expression as follows:

$$\begin{aligned}&|\mathrm{Im}f(z)-\mathrm{Im}g(z)|\\&\leq\max|\mathrm{Im}f-\mathrm{Im}g|\,\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}[\tan\mu(y)-\tan\gamma(x)]\\&\times2\left(\frac{d\sigma}{d\Omega}(y)\right)^{1/2}\frac{\Theta(K)}{K^{1/2}}\,dx\,dy.\end{aligned} \tag{9}$$

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The uniqueness condition becomes

$$\frac{q}{2\pi}\int_{-1}^{+1}\int_{-1}^{+1}[\tan\mu(y)-\tan\gamma(x)]\,2\,|f(y)|\,\frac{\Theta(K)}{K^{1/2}}\,dx\,dy<1, \tag{10}$$

where we could equally well write $|g(y)|$ since $|f(y)| = |g(y)|$. Everything in this expression is known in terms of the given modulus of the amplitude. Since the values of the modulus at all points are used to find both $\mu(y)$ and $\gamma(x)$ and also to evaluate the integral (unlike in our previous uniqueness condition where only the supremum and infinum values were used), this uniqueness condition cannot be directly compared with our previous result without a knowledge of $|f(z)|$. This is because of the different ways the integrands were majorized. Whereas the modulus is a bad majorization for the real part, the angle-dependent upper and lower bounds are definite improvements over the supremum and infinum. Another uniqueness condition which follows from Eq. (8) is

$$\tan y\mu - \tan\gamma_{\min} < 1.$$

This has the same form as Eq. (22) of Ref. 1, but $\Theta_{\min}$, which is obtained in terms of ν and $y\mu$, is replaced by $\gamma_{\min}$ which is likely to be a better lower bound.

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Topological solitons and graded Lie algebras

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This paper is an extension of our previous investigation on the crossing of defects in ordered media. We provide a general mathematical framework, in which the obstructions for crossing p-dimensional defects with q-dimensional defects in a $(p+q+1)$-dimensional sample are the brackets of a certain graded Lie algebra (connected with homotopy theory). This "confinement mechanism" brings together the mathematical structures of two not yet related themes in present-day physics: solitons and supersymmetry.

INTRODUCTION

In a previous paper we have used topological concepts and methods applied to problems in solid state physics.[1] Our study belonged to the framework of the physical theories which classify stable defects in ordered media in terms of homotopy groups of a "manifold of internal states" V (characteristic for the type of order under consideration). See Refs. 1–4 and also Ref. 5.

In Ref. 1 we showed that noncommutation relations in $\pi_1 V$ have as effect a sort of "entanglement": Defect lines in three-dimensional samples of the ordered medium cannot cross each other. In the present paper we show that a similar "confinement mechanism" works in higher dimensions. More exactly, the obstructions for crossing "defect hypersurfaces" of dimension p and q in a $(p+q+1)$-dimensional sample are the brackets in a certain graded Lie algebra connected to the homotopy groups of V. These brackets are the well-known Whitehead products

$$\pi_p V \times \pi_q V \xrightarrow{[,]} \pi_{p+q-1} V$$

from homotopy theory. These brackets are exactly the commutators if $p=q=1$; one can always think of them as commutators in an enveloping algebra. In the crucial four-dimensional case the vanishing of our brackets just means that the action of $\pi_1 V$ on $\pi_2 V$ is trivial.

So, anyway, here is a "confinement mechanism" which again, as in the three-dimensional case of biaxial nematics[1] depends on some noncommutativity relation. Strangely too, this brings together two, until now, unrelated themes of modern physics: solitons (i.e., homotopy) and supersymmetry (i.e., graded Lie algebras).

1. REVIEW OF WHITEHEAD PRODUCTS

In this section we will recall (without proofs) whatever is necessary to know about Whitehead products, in homotopy theory, for the rest of the paper. For more details we refer to Refs. 6 and 7. We believe that Whitehead products should become a familar notion to physicists interested in supersymmetry and (topological) solitons.

Let (X,x_0) be an arcwise connected space with base point x_0. For $p,q \geq 1$ we define maps

$$\pi_p(X,x_0)\times\pi_q(X,x_0) \to \pi_{p+q-1}(X,x_0)$$

which with $\alpha \in \pi_p$, $\beta \in \pi_q$ associate their "Whitehead product" $[\alpha,\beta] \in \pi_{p+q-1}$, as follows.

We start by considering the unit cubes in the Euclidean spaces R^p, R^q,

$$I^p \subset R^p = \{(t_1,\ldots,t_p)\},\quad I^q \subset R^q = \{(u_1,\ldots,u_q)\}.$$

The unit p-cube with the boundary crushed to a point, $I^p/\partial I^p$, is the sphere S^p (endowed with a base point $*_p =$ the image of ∂I^p, and with an orientation coming from the "standard" orientation of R^p). [*Remark*: So, we have a natural projection $I^p \xrightarrow{\pi_p} I^p/\partial I^p = S^p$ and, if $t \in I^p$ we will think of t as being a (singular) "coordinate system" on S^p and write t instead of $\pi_p(t)$.] Inside of $S^p \times S^q$ we consider $S^p \vee S^q =$ (the S^p-factor $\times$ the base point of S^q) $\cup$ (the base point of $S^p \times$ the S^q-factor) $\subset S^p \times S^q$.

Let $\partial(I^p \times I^q) = \partial I^p \times I^q \cup I^p \times \partial I^q$ (with the two copies of $\partial I^p \times \partial I^q$ coming from $\partial I^p \times I^q$, $I^p \times \partial I^q$ identified), endowed with the base point $(0,0)$, and

$$w_{p,q}: [\partial(I^p \times I^q), (0,0)] \to [S^p \vee S^q, (*_p, *_q)]$$

defined as follows:

$$w_{p,q}(t,u) = \begin{cases} (t, *_q) & \text{if } t \in I^p,\ u \in \partial I^q, \\ (*_p, u) & \text{if } t \in \partial I^p,\ u \in I^q. \end{cases}$$

Note that one gets $S^p \times S^q$ by gluing $I^p \times I^q$ to $S^p \vee S^q$ along $w_{p,q}$.

Let f: $(S^p, *_p) \to (X,x_0)$, g: $(S^q, *_q) \to (X,x_0)$ be continuous maps which represent the elements

$$\alpha \in \pi_p(X,x_0),\quad \beta \in \pi_q(X,x_0).$$

We orient I^p, I^q canonically, $I^p \times I^q$ receives the product orientation, and $S^{p+q-1} = \partial(I^p \times I^q)$ will be oriented accordingly.

The map

$$S^{p+q-1} = \partial(I^p \times I^q) \xrightarrow{w_{p,q}} S^p \vee S^q \xrightarrow{f \vee g} X$$

respects the base points. Its (based) homotopy class depends only on α, β and is, by definition,

$$[\alpha,\beta] \in \pi_{p+q-1}(X,x_0).$$

Remark: A very useful description of the *free*

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homotopy class $[\alpha,\beta]$ is the following: Consider oriented copies of S^p, S^q and orient $S^p\times S^q$ accordingly. Consider N^{p+q} = a smooth regular neighborhood of $S^p\vee S^q\subset S^p\times S^q$, with the induced orientation, and some retraction $N^{p+q}\xrightarrow{r} S^p\vee S^q$. Orient $S^{p+q-1}=\partial N^{p+q}$ like $-N^{p+q}$. The (free) homotopy class of

$$\partial N^{p+q}\xrightarrow{r} S^p\vee S^q\xrightarrow{f\vee g} X$$

is $[\alpha,\beta]$ (considered as a *free* homotopy class).

Here is a list of some elementary properties of the Whitehead product; as usual, the composition law of π_i is written multiplicatively if $i=1$ and additively if $i>1$.

(1) Let $\alpha\in\pi_1(X,x_0)$, $\beta\in\pi_1(X,x_0)$. Then

$$[\alpha,\beta]=\alpha\beta\alpha^{-1}\beta^{-1}\in\pi_1(X,x_0).$$

So in dimension one, the Whitehead product is just the commutator. This fits beautifully with the next properties which show that the Whitehead product is always a sort of a commutator product.

(2) Let $p, q, r>1$ and

$$\alpha\in\pi_p,\quad \beta\in\pi_q,\quad \gamma\in\pi_r.$$

Then

$$[\alpha,\beta]=(-1)^{pq}[\beta,\alpha]\ \text{(anticommutativity)},$$

and

$$(-1)^{qr}[\alpha,[\beta,\gamma]]+(-1)^{rp}[\beta,[\gamma,\alpha]]+(-1)^{pq}[\gamma,[\alpha,\beta]]=0.$$

The last formula is the "graded form" of the Jacobi identity. Moreover, if $p, q>1$, $[\alpha,\beta]$ depends bilinearly on α and β.

In other words, if we consider the graded Abelian group

$$\pi_{*+1}(X,x_0)=\sum_{p=1}^{\infty}M_p,$$

where $M_p=\pi_{p+1}(X,x_0)$, together with the Whitehead product

$$M_p\otimes M_q\xrightarrow{[\,,\,]} M_{p+q}$$

we obtain a *graded Lie algebra*. (See Ref. 8 for the general properties of graded Lie algebras and their relations to physics. The graded algebras under consideration here are Z algebras).

Comment: Let ΩX be the "loop space" of X (based at x_0). ΩX has a natural product which makes it an (associative) H space, and $\pi_p(X)=\pi_{p-1}(\Omega X)$ (see for instance Ref. 7).

Even better, in the semisimplicial context, ΩX is interpreted as a semisimplicial group (see for instance Ref. 9). Anyway, there is a continuous, "grouplike," composition law

$$\Omega X\times\Omega X\to\Omega X$$

and the induced map

$$\pi_{p-1}(\Omega X)\times\pi_{q-1}(\Omega X)\to\pi_{p+q-2}(\Omega X)$$

is our Whitehead product.

Roughly speaking $\pi_{*+1}(X)$ is for this very large grouplike object what a standard Lie algebra is for a usual Lie group. Somehow, the idea is that *graded* Lie algebras are the infinitesimal (super)symmetries coming from really "very large groups."

The fundamental group of X is the group of connected components of ΩX $[\pi_1X=\pi_0(\Omega X)]$. Remember also that π_1 acts naturally on π_p. For $p=1$ this is just the natural action by inner automorphism. If $p>1$, π_p has a natural π_1 module structure. [This means that for $\alpha\in\pi_1(X,x_0)$, $\beta\in\pi_p(X,x_0)$ an element $\alpha.\beta\in\pi_p(X,x_0)$ is defined; the operation $\pi_p\xrightarrow{\alpha.}\pi_p$ is an automorphism and $\alpha'.(\alpha.\beta)=(\alpha'.\alpha).\beta$. One should think of this operation as the natural generalization of the operation of π_1 on itself by inner automorphism. Again see Ref. 7, or any standard text for details.]

(3) If $\alpha\in\pi_1(X,x_0)$, $\beta\in\pi_p(X,x_0)$ $(p>1)$,

then

$$[\beta,\alpha]=\beta-\alpha.\beta,\ \text{and}\ [\alpha,\beta]=(-1)^p(\beta-\alpha.\beta).$$

(4) If $[\alpha,\beta]=0$, the same is true if one changes the order of factors or their orientations.

(5) If $\phi\colon (X,x_0)\to(Y,y_0)$ is a continuous map and $\alpha\in\pi_p(X,x_0)$, $\beta\in\pi_q(X,x_0)$, then

$$\phi_*[\alpha,\beta]=[\phi_*\alpha,\ \phi_*\beta]\in\pi_{p+q-1}(Y,y_0).$$

(6) Let f,g represent α,β. Then $[\alpha,\beta]=0$ if and only if $f\vee g\colon S^p\vee S^q\to X$ extends to a continuous map $S^p\times S^q\to X$.

Remark: If X is an H space, i.e., if it is endowed with a continuous multiplication for which the base point is a homotopy identity), then all the Whitehead products vanish. The converse is also true in the case of spheres; actually the only spheres which are H spaces are S^0, S^1, S^3, and S^7 (see Ref. 10).

2. A MODEL FOR HIGH-DIMENSIONAL ORDERED MEDIA; STATEMENT OF THE MAIN RESULT

We give now a topological model for a "high-dimensional ordered medium." This is a direct generalization of our three-dimensional model given in Ref. 1, and the reader who would feel a need for an exposition of the concepts at a more elementary level with examples and drawings is advised to consult that reference.

The model consists of the following data:

(1) A topological space V, called the "*manifold of internal states.*" For simplicity's sake, we will assume V to be connected. For instance, in a three-dimensional isotropic ferromagnet, this manifold V is the two-dimensional sphere, corresponding to all possible orientations of the magnetic moment, characterizing the internal magnetic state.

(2) An n-dimensional smooth manifold M^n, called the "*physical space.*" The physical space is the space of the medium: For material samples, generally $n=3$. Again, for simplicity, M^n is supposed connnected and without boundary. M^n and V will be fixed, once and for all.

(3) Our "*ordered medium*" will be a pair (Σ,Φ) where Σ is a subset of M^n and

$$M^n-\Sigma\xrightarrow{\Phi} V$$

is a continuous map, assigning to every $p \in M^n - \Sigma$ an "*order parameter*" $\Phi(p) \in V$. For instance, in a three-dimensional isotropic ferromagnet, the order parameter is the magnetic moment and Σ is the locus of points in the medium where the orientation of the magnetic moment is not well defined (locus of singularities of the order parameter). The subset Σ, which is the "*set of defects*," will be assumed to be a compact submanifold with boundary, of dimension n. Generically, Σ will be supposed to possess a spine Γ (which means a polyhedron contained in the interior of Σ such that Σ' is obtained by thickening Γ to a smooth submanifold of codimension 0 of M^n) of dimension $\leq k$, where $k = [n - (\text{the lowest } i \text{ such that } \pi_i V \neq 0) - 1]$. From a physical standpoint this is a very natural assumption (see Refs. 1,2 and 4). It will be convenient to assume that Φ is defined not only on $M^n - \Sigma$ but also on $\partial\Sigma =$ the boundary of Σ; of course we could as well consider a Φ defined on $M^n - \Gamma$ but it is more convenient to state our results in terms of a smooth set of defects.

We shall consider three kinds of *elementary operations* which transform one ordered medium (Σ, Φ) into another (Σ', Φ').

(0) *Isotopy* (i.e., "moving things around"): This means that we consider a 1-parameter family of diffeomorphisms of the physical space $\Phi_t : M^n \to M^n$ such that $t \in [0,1]$, Φ_0 is the identity, and $\Sigma' = \Phi_1 \circ \Sigma$, $\Phi' = \Phi \circ \Phi_1$.

(1) *Positive surgery of index* λ: We consider a smoothly embedded n-ball $D^n = D^\lambda \times D^{n-\lambda} \subset M^n - \text{int}\Sigma$, such that

$$D^n \cap \partial\Sigma = \partial D^n \cap \partial\Sigma = \partial D^\lambda \times D^{n-\lambda}.$$

We can define a new ordered medium

$$\Sigma' = \Sigma \cup (D^\lambda \times D^{n-\lambda}), \quad \Phi' = \Phi \,|\, M^n - \text{int}\Sigma'.$$

Remarks: (a) Remember that

$$\partial(D^\lambda \times D^{n-\lambda}) = \partial D^\lambda \times D^{n-\lambda} \cup D^\lambda \times \partial D^{n-\lambda},$$

where the two terms of the right-hand side are glued together along the common $\partial D^\lambda \times \partial D^{n-\lambda-1} = \partial(\partial D^\lambda \times D^{n-\lambda}) = \partial(D^\lambda \times \partial D^{n-\lambda})$. The new Σ' is obtained by gluing Σ and $D^\lambda \times D^{n-\lambda}$ along $\partial D^\lambda \times D^{n-\lambda}$ and smoothing the result. One says that Σ' is obtained from Σ by *adding a handle of index* λ.

(b) Up to isotopy the passage from the submanifold Σ to the submanifold Σ' is completely determined by the λ-ball $D^\lambda \times$(the center of $D^{n-\lambda}$). Notice that (up to homotopy) there is only one trivialization of the normal bundle of ∂D^λ in $\partial\Sigma$ which extends to a trivialization of the normal bundle of $D^\lambda \times$(center of $D^{n-\lambda}$) in M^n.

(c) The fact that Σ has a spine of dimension $\leq k$ means exactly that Σ is obtained from $\emptyset \subset M^n$ by adding handles of index $\leq k$.

(2) *Negative surgery of index* λ: We consider a ball of dimension λ D^λ embedded smoothly in Σ, in such a way that $\partial D^\lambda = D^\lambda \cap \partial\Sigma$ meeting $\partial\Sigma$ transversally. One can extend D^λ to an embedding $D^\lambda \times D^{n-\lambda} \subset \Sigma$ such that D^λ is identified to $D^\lambda \times$(center of $D^{n-\lambda}$), with $\partial(D^\lambda \times D^{n-\lambda}) \cap \partial\Sigma = (D^\lambda \times D^{n-\lambda}) \cap \partial\Sigma = \partial D^\lambda \times D^{n-\lambda}$. Then one can "cut Σ along D^λ" and define

$$\Sigma' = \Sigma - D^\lambda \times \text{int}D^{n-\lambda}$$

(which, up to isotopy, is completely determined by D^λ). Assume now also that

$$[\Phi \,|\, \partial D^\lambda] = 0 \in \pi_{\lambda-1} V.$$

Then there are extensions of Φ to $M^n - \Sigma'$; call Φ' such an extension. We have obtained a new ordered medium (Σ', Φ').

Remarks: One can think of $[\Phi \,|\, \partial D^\lambda]$ (element of $\pi_{\lambda-1} V$, well defined only up to the action of some element of $\pi_1 V$) as being the "physical obstruction" for realizing the negative surgery. Of course, no such obstructions exist for positive surgery.

In physical terms, one should always think of the points of Σ as being at higher energy level than the rest of M^n. So there is a "core energy" proportional to the "size" of the set of defects and this energy will tend to be spontaneously reduced. This means that negative surgery will tend to happen all by itself while positive surgery (as well as isotopies streching Σ) need an input of energy from outside. Again, in principle, positive surgery of higher index should require a larger energy input of energy than positive surgery of lower index. With a very large input of energy one could excite all of M^n (hence make $M^n = \Sigma$, which is very nongeneric) and hence pass from any (Σ, Φ) to any other (Σ', Φ').

On the other hand, our surgery operations (and the isotopy) are the minimal geometric changes one can make on the set of defects. If one introduces outside energy "petit à petit," by small amounts, the kind of deformations of the set of defects one should expect are isotopies and surgeries.

We consider now a less "elementary" deformation of Σ. Start with a handle decomposition of Σ, and let $D^p \times D^{n-p}$, $D^q \times D^{n-q}$ be two handles of this decomposition, such that

$$p + q = n - 1.$$

We shall define a purely topological operation (no Φ involved) of *Crossing a p-handle with a q-handle*.

It is convenient now to think of Σ as being obtained by thickening some spine Γ such that the balls $D^p = D^p \times$(center of D^{n-p}) and $D^q = D^q \times$(center of D^{n-q}) are contained in Γ (in such a way that int D^p, int D^q are *open* subsets of Γ). Let $*_p \in D^p$, $*_q \in D^q$ be the centers of the corresponding balls and consider a smoothly embedded line segement

$$[0,1] \xrightarrow{L} M^n$$

such that $L(0) = *_p$, $L(1) = *_q$; $L(0,1) \cap \Gamma = \emptyset$, $L[0,1]$ is *not* tangent to D^p or D^q. Without any loss of generality, assume that M^n has a Riemannian metric such that L and D^p (respectively D^q) are actually orthogonal.

By definition, an *infinitesimal crossing data* is a trivialization of the normal bundle of L in M^n,

$$\nu L \xrightarrow{\theta} R^{n-1}$$

such that $\theta(T_{*_p} D^p)$ and $\theta(T_{*_q} D^q)$ are *transversal*. Two infinitesimal crossing data

$$\nu L \underset{\theta_1}{\overset{\theta_0}{\rightrightarrows}} R^{n-1}$$

are, by definition, *homotropic*, if there is a homotopy of trivializations,

$$\nu L \xrightarrow{\theta_t} R^{n-1}$$

connecting them so that $\theta_t(T_{*_p}D^p)$, $\theta_t(T_{*_q}D^q)$ stay transversal for all $t \in [0,1]$.

If $n \geq 4$ there are exactly four distinct homotopy classes of infinitesimal crossing data. To see this it is better to give an equivalent but asymmetric form of the definition of our infinitesimal crossing data. Instead of a θ as before we consider a trivialization

$$\nu L \xrightarrow{\theta'} \nu_{*_p} L \supset T_{*_p} D^p$$

such that $\theta'(T_{*_q}D^q)$ and $T_{*_p}D^p$ are transversal.

Then, one can perturb a given θ' by changing via a "half-twist" the orientation of $\theta'(T_{*_q}D^q) \approx (T_{*_p}D^p)^\perp$, or by combining θ' (via a "full twist") with the unique non-trivial element of $\pi_1\,\mathrm{SO}(n-1) = Z/2$, or by doing simultaneously both operations described. It is an easy exercise to prove that in this way we get exactly all the homotopy classes. Of course, if $n=3$ there are infinitely many classes [since $\pi_1\,\mathrm{SO}(2) = Z$]. The situation for $n=3$ is described by pictures in Ref. 1.

A *crossing data* is, by definition, a local chart

$$R^n \xrightarrow{\psi} M^n$$

such that $R^n = \{(x_1, \ldots, x_p, y_1, \ldots, y_q, z)\}$ and

(a) $\psi(R^n) \cap (\Gamma \cup L) = L \cup$ (a small open p-ball in D^p) $\cup$ (a small open q-ball in D^q),

(b) $\psi^{-1}(L) = \{x = y = 0,\ -1 \leq z \leq 1\}$,

(c) $\psi^{-1}(D^p) = \{y = 0,\ z = 1\}$,

(d) $\psi^{-1}(D^q) = \{x = 0,\ z = -1\}$.

Two crossing data are isotopic (by definition) if the germs of $(x=0)$, $(y=0)$ along L vary by isotopy, staying transversal. There is a natural bijection between homotopy classes of infinitesimal crossing data and isotopy classes of crossing data. This is quite clear intuitively, and not hard to prove, anyway.

Given a "crossing data" we can use it in order to change the position of Σ in M^n to a new $\Sigma_\psi \subset M^n$, obtained by letting $D^p(D^q)$ cross $D^q(D^p)$ along L, staying in the "plane" $\psi(y=0)$ [respectively $\psi(x=0)$]. The two results are isotopic in M^n so there is no difference whether D^p crosses D^q or D^q crosses D^p. {The formal definition goes as follows: One considers a smooth function $z = h(y)$ such that $h(0) > 1$, $h(y) = -1$ if $|y|$ is large and one replaces D^q by $\psi\{x=0,\ z=h(y)\}$.}

Σ_ψ is hence just the image of another smooth embedding $\Psi: \Sigma \to M^n$. The isotopy class of Ψ depends only on the isotopy class of ψ.

Now, consider $x_0 = L(1/2)$ and two small balls: Δ^{q+1} of center $*_p$, orthogonal to D^p and Δ^{p+1} of center $*_q$, orthogonal to D^q. By orienting (in any arbitrary way) $\partial\Delta^{q+1}$ $(\partial\Delta^{p+1})$ and joining them to x_0 along L by the obvious paths one obtains two elements

$$\alpha_p \in \pi_p(M^n - \Sigma, x_0), \quad \beta_q \in \pi_q(M^n - \Sigma, x_0).$$

We shall consider the Whitehead product

$$\Phi_*[\alpha_p, \beta_q] = [\Phi_*\alpha_p, \Phi_*\beta_q] \in \pi_{p+q-1}V = \pi_{n-2}V.$$

We can now state our

Main result: Let (Σ, Φ) be an ordered medium and ψ a crossing data giving rise to $\Sigma_\psi \subset M^n$. The following two conditions are equivalent:

(1) There is an ordered medium (Σ_ψ, Φ') such that one can go from (Σ, Φ) to (Σ_ψ, Φ') by a finite sequence of operations of the following type:

(1a) isotopy.

(1b) negative surgery.

(1c) positive surgery of index $\lambda = 0, 1$.

(1d) positive surgery of index $\lambda \geq 2$, not touching (a neighborhood of) L.

(2) $[\Phi_*\alpha_p, \Phi_*\beta_q] = 0 \in \pi_{p+q-1}(V)$.

In particular, if ψ_1, ψ_2 are two crossing data corresponding to the same L, one can pass from (Σ, Φ) to some $(\Sigma_{\psi_1}, \Phi_1')$, by operations (1a)–(1d) if and only if one can pass to some $(\Sigma_{\psi_2}, \Phi_2')$ (by the same kind of operations). □

The proof will be given in the next section.

Remarks: I The three-dimensional case $(p=q=1)$ of this theorem is covered by our previous result.[1] Also Ref. 1 contains several drawings which might help understanding the next paragraph.

II. If $p+q \leq n-2$ there is no obstruction whatsoever for crossing. (It can be done by isotopy; see also our last paragraph).

III. If $p+q=n$ the problem is very different: One wants to get rid of (isolated) intersection points between a p-dimensional cell of Γ and a q-dimensional one. In "high dimensions" $(p \geq 3,\ q \geq 3)$ this is taken care of by classical arguments: Whitney for the case $\pi_1 M^n = 0$ (see Refs. 11 and 12 or Kervaire in the nonsimply connected case.[13]) If $n=4$, $p=q=2$ the problem is largely beyond the present state of the art. (See however the more or less recent results of Casson.[14])

IV. Only the positive surgery of index $\leq k$ is "physically relevant."

3. PROOF OF THE MAIN RESULT

We consider

$$R^p = \{(x_1, \ldots, x_p)\}, \quad R^q = \{(y_1, \ldots, y_q)\}$$

with their canonical orientations,

$$R^n = R^{p+q+1} = \{(x_1, \ldots, x_p, y_1, \ldots, y_q, z)\}$$

and the linear subvarieties (of R^n)

$$Y = \{x = 0,\ z = -1\}, \quad X_t = \{y = 0,\ z = t\}.$$

The z axis, $R = \{x = y = 0\}$ is oriented canonically. We consider, like in the previous paragraph, small disks: $\Delta^{q+1} \subset \{x=0\}$, oriented like $(-R)\times R^q$, centered at $(x=0,\ y=0,\ z=1)$ and $\Delta^{p+1} \subset \{y=0\}$ oriented like $R \times R^p$, centered at $(x=0,\ y=0,\ z=-1)$. Their oriented boundaries give rise to well-defined elements,

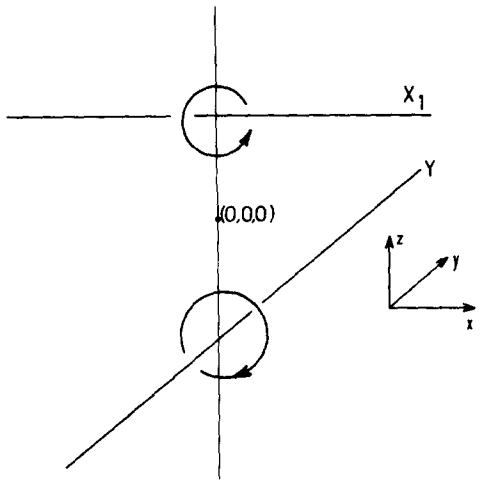

FIG. 1.

$$\alpha_p \in \pi_p(R^n - X_1 - Y), \quad \beta_q \in \pi_q(R^n - X_1 - Y),$$

defined as in the previous section (except that now we have fixed their signs). So we have a well-defined element

$$[\alpha_p, \beta_q] \in \pi_{p+q-1}[R^n - X_1 - Y, (0,0,0)].$$

In Fig. 1, we have represented X_1 and Y in the three-dimensional case, where $p=q=1$. In Fig. 2, we show what happens after X_1 has crossed Y, along the z axis, staying in the plane $y=0$. We achieve this by changing X_1 into X'_{-2} where X'_{-2} looks like X_{-2} in the neighborhood of the z axis, and like X_1 in the neighborhood of infinity.

[*Remark*: Up to isotopy, there is no difference in between $X'_{-2} \cup Y \subset R^3$ and $X_{-2} \cup Y \subset R^3$.]

Let $Z_t = X_t \cup Y \cup R$ and $U_t = R^n - Z_t$. Consider now t_0, $t_1 \in R$ and K some (let's say compact) topological space. If $f: K \to U_{t_0}$ is a continuous map, one can always construct another continuous map $F: K \times [t_0, t_1] \to R^n \times [t_0, t_1]$, commuting with the projection on the $[t_0, t_1]$ factor, such that $F(K \times t) \subset U_t$, $F \mid K \times t_0 = f$. (The reader should think of the "continuous operation" which changes Z_{t_0} into Z_t by sliding X_{t_0} along R, and, corresponding to this continuous deformation, the operation of pushing $f(K)$ into U_t.)

It is easy to see that the homotopy class of $K = K \times t_1 \xrightarrow{F_{t_1}} U_{t_1}$ depends only on the homotopy class of f. In this way we get a canonical homotopy equivalence (well determined up to homotopy)

$$H_{t_0, t_1}: U_{t_0} \to U_{t_1}.$$

In U_{-2} we consider the homotopy class $f: S^{n-2} \to U_{-2}$

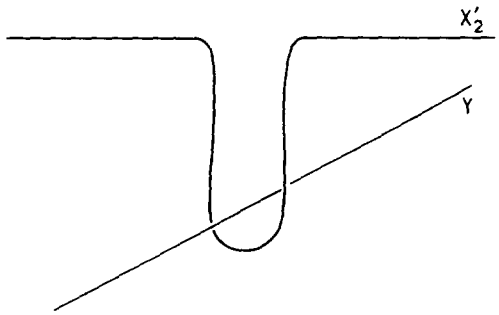

FIG. 2.

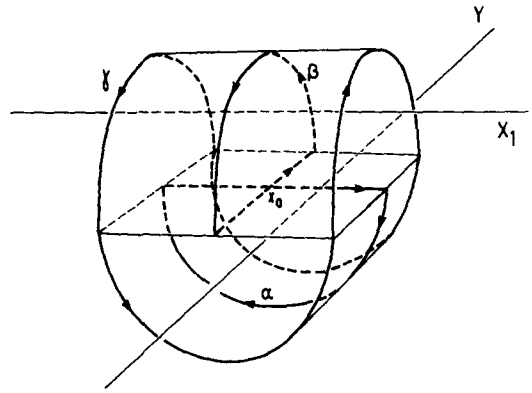

FIG. 3.

defined as follows: In the plane $z = -\frac{3}{2}$ consider the polydisk:

$$\Delta^{n-1} = \{\Sigma x_i^2 \leq 5, \ \Sigma y_j^2 \leq 5\},$$

oriented like $R^p \times R^q$. The boundary $\partial \Delta^{n-1} = [(\Sigma x_i^2 = 5) \times (\Sigma y_j^2 \leq 5)] \cup [(\Sigma x_i^2 \leq 5) \times (\Sigma y_j^2 = 5)]$ with its induced orientation, can be though of as a homotopy class $S^{n-2} \to U_{-2}$, which is, by definition, our f.

Lemma A: The map $S^{n-2} \to R^n - X_1 - Y$ defined by the composition

$$S^{n-2} \xrightarrow{f} U_{-2} \xrightarrow{H_{-2,1}} U_1 \xrightarrow{i} R^n - X_1 - Y$$

is in the same (free) homotopy class as the Whitehead product

$$[\alpha_p, \beta_q]: S^{n-2} \to R^n - X_1 - Y.$$

Proof: Consider the following two subsets of $R^n - X_1 - Y$

$$A = (\Sigma x_i^2 \leq 5) \times [(\Sigma y_j^2 + z^2 = 5, \ z > 0) \cup (\Sigma x_k^2 \leq 5, \ z = 0)],$$

$$B = (\Sigma y_j^2 \leq 5) \times [(\Sigma x_i^2 + z^2 = 5, \ z < 0) \cup (\Sigma x_k^2 \leq 5, \ z = 0)].$$

Clearly $A \cap B = \Delta^{n-1} \times (z = 0)$ and moreover $C = A \cup B$ is a piecewise differentiable submanifold with boundary, of dimension $n-1$ in $R^n - X_1 - Y$, homeomorphic to $S^p \times S^q$ – {the interior of a smoothly embedded $(n-1)$-ball}. Our Fig. 3 represents C in the three-dimensional case, $p=q=1$. $A \cap B$ is now the square

$$\{-1 \leq x \leq 1, \ -1 \leq y \leq 1, \ z = 0\}$$

and our base point x_0 is the center of this square. Contained in C are three oriented curves, drawn in fat lines α, β, γ. α and β are respectively representatives of $\alpha_1 \in \pi_1(R^3 - X_1 - Y)$ and $\beta_1 \in \pi_1(R^3 - X_1 - Y)$. Moreover, γ is in the same *free* homotopy class as the commutator $[\alpha_1, \beta_1]$. Properties (0)–(4) listed below should be intuitively clear in this picture.

We can also observe the following facts:

(0) $\partial C = [\Sigma x_i^2 = 5, \ \Sigma y_i^2 + z^2 = 5, \ z \geq 0]$

$$\cup [\Sigma x_i^2 + z^2 = 5, \ \Sigma y_i^2 = 5, \ z \leq 0]$$

(the intersection of the two terms of the right-hand side being $[\Sigma x_i^2 = 5, \ \Sigma y_i^2 = 5, \ z = 0]$).

(1) The projection $R^n = R^p \times R^q \times R \xrightarrow{\pi} R^p \times R^q$ induces a homeomorphism

$$\partial C \xrightarrow{\pi} \partial \Delta^{n-1}.$$

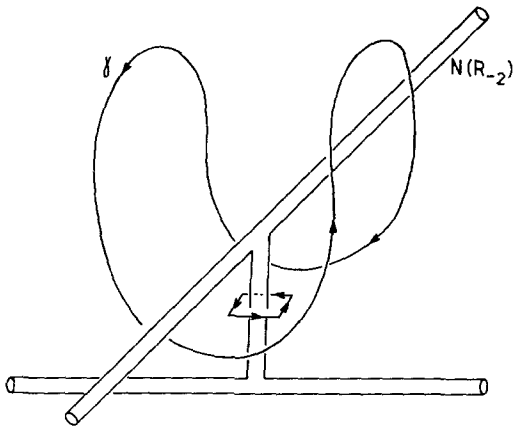

FIG. 4.

(2) If we orient $\partial\Delta^{n-1}$ as before and give ∂C the induced orientation via π, then ∂C (considered as a continuous map $S^{n-2} \to R^n - X_1 - Y$) is in the same (free) homotopy class as $[\alpha_p, \beta_q]$.

(3) If $t \in [-2,1]$, $\partial C \cap Z_t = \phi$.

(4) If $P \in \partial C$, the line segment joining P to $(\pi(P), z = -\frac{3}{2})$ does not touch Z_{-2}. In particular, in U_{-2}, ∂C is in the same homotopy class as f: $S^{n-2} \to U_{-2}$.

All these facts together, imply our *Lemma* A.

Remark 1: The exact signs in the previous considerations are immaterial for the rest of the proof. All we need is that

$$[\alpha_p, \beta_q] = \pm i \circ H_{-2,1} \circ [f] \quad \text{(free homotopy)}.$$

Remark 2: If we define $Z'_t = X_t \cup Y \cup [x = y = 0, z \in [t, -1]]$, $U'_t = R^n - Z'_t$ we can define homotopy equivalences $H'_{t_0,t_1}: U'_{t_0} \to U'_{t_1}$ as above and prove an analogous lemma.

Remark 3: If D^p, D^q are oriented, and are joined by L, and if a crossing data ψ is given, we have constructed an element $[\alpha_p, \beta_q] \in \pi_{p+q-1}(M^n - \Sigma)$ which *a priori* depends on the various choices of orientations and on the homotopy class of L. It is easy to see that it actually does *not* depend on ψ. This, together with the rest of this section proves the last sentence of our main result.

Lemma B: (1) $\Rightarrow$ (2) □

Proof: Without any loss of generality $\partial C \subset M^n - \Sigma$. Moreover, any time one passes from (Σ, Φ) to $(\tilde{\Sigma}, \tilde{\Phi})$ by one of the operations (1a)–(1d) one can still assume that ∂C stays outside $\tilde{\Sigma}$.

For (1a), (1b) this is obvious; for (1c) it follows from general position since $\dim \partial C = n - 2$; for (1d) it follows from the assumption that the corresponding surgery does not touch L (and hence ∂C).

So we can assume that $\Phi \mid \partial C = \Phi' \mid \partial C$. But then Lemma A shows that ∂C is null-homotopic in $M^n - \Sigma_\psi$. Hence

$$\Phi_*[\alpha_p, \beta_q] = [\Phi \mid \partial C] = [\Phi' \mid \partial C] = 0 \in \pi_{p+q-1}(V).$$

This proves that (1) $\Rightarrow$ (2).

Lemma C: If $\Phi_*[\alpha_p, \beta_q] = 0 \in \pi_{p+q-1}(V)$ one can pass from (Σ, Φ) to an ordered medium of the form (Σ_ψ, Φ') by one positive surgery of index 1 followed by one negative surgery of index $n-1$, and isotopies. □

Proof: With the notation from the begining of this section, consider $X_1 \cup Y$ as part of (the spine of) Σ and $X_{-2} \cup Y$ as part of (the spine of) Σ'. Call the corresponding spines Γ, Γ_{-2}. We can consider a positive surgery of index 1 which goes from (Σ, Φ) to

$$\Sigma_1 = \Sigma + (\text{a handle of index 1 along } L),$$

$$\Phi_1 = \Phi \mid \Sigma_1.$$

Σ_1 has a spine $R_1 = \Gamma$ with $X_1 \cup Y$ replaced by Z'_1 (see Remark 2, after Lemma A). We can also consider $R_t = \Gamma$ with $X_1 \cup Y$ replaced by Z'_t. Let $N(R_t)$ be a regular neighborhood of R_t in M^n. So $N(R_1) = \Sigma_1$ and $N(R_t)$ varies by isotopy. One has an isotopy of ordered media

$$[N(R_t), \Phi_t] \quad (N(R_t) = \text{the set of defects}),$$

with t varying from $+1$ to -2.

One can go from $N(R_{-2})$ to Σ' by one negative surgery represented by cutting exactly along $\Delta^{n-1} \times (z = -\frac{3}{2})$, and isotopies. For this surgery to be "physically realizable" one has to have $\Phi_{-2}\{\partial[\Delta^{n-1} \times (z = -\frac{3}{2})]\} = 0$ [in $\pi_{p+q-1}(V) = \pi_{n-2}(V)$]. But by Lemma A this is equivalent to $\Phi_*[\alpha_p, \beta_q] = 0$. And so the proof is finished. The argument is shown pictorially in Fig. 4. The point is that in $R^3 - N(R_{-2})$, the curve γ (from Figs. 3 and 4) and $\partial[\Delta^2 \times (z = -\frac{3}{2})]$ with the good orientation are homotopic.

4. BRIEF PHYSICAL CONSIDERATIONS

Topological solitons are of interest in two different domains of physics. In condensed matter physics, in order to describe defects or textures of ordered media. In relativistic field theory, in order to describe particles or pseudoparticles (instantons).

For the physics of condensed matter, the canonical dimensionality to be considered is dimension three. This situation is discussed in detail in our previous paper.[1]

In relativistic field theory, however, the canonical dimensionality is four and this was one of our motivations for extending the analysis to arbitrary dimension. Another motivation is that in this more general context the real issues, in particular the connection with graded Lie algebras, become clearer. It should be mentioned here, that in the present field theory models, involving topological solitons, the manifold of internal states V is generally a Lie group G; in such a situation our present paper shows that there are no topological obstructions to crossing, since all the Whitehead products vanish.

It is worth recognizing that these obstructions to crossing lead naturally to a confinement mechanism. For instance, in dimension three, if one closed string is entangled with another closed string, and if there is an obstruction to crossing due to the noncommutativity of π_1, separating one string from another (assuming that each one has a given size) will cost an energy increasing linearly with distance, due to the creation of extra defect volume connecting the two strings.

Similarly, in dimension four, if π_1 acts nontrivially on π_2 one has obstructions for disentangling closed strings

from "bags." In this sense entanglement leads to confinement; this paper provides the theory for the entanglement of a p-defect with a q-defect in a space of dimension $d = p + q + 1$.

In the Appendix of our first paper we have discussed the interaction of two punctual defects in dimension two. If $\pi_1 V$ is noncommutative the way such defects interact may depend on the path followed to join them: For instance two point defects may annihilate each other if they are joined along some path and *not* if they are joined along some other path.

In a space of dimension d, a point defect (described by π_{d-1}) turning around a defect of codimension 2 (described by π_1) may find its topological character changed, if π_1 acts nontrivially on π_{d-1}. And again, two point defects may annihilate along some path and not along some other [the simplest materials where this effect might be observed are the ordinary (uniaxial) nematic liquid crystals, for which $V = P_2$, the projective plane]. Note that, in these situations, one is considering the interaction of a p-defect and q-defect, with $p = 0$, $q = d - 2$ and $p + q = d - 2$. (See also Ref. 5.)

It looks as if all the algebraic structures built in homotopy theory lead to simple physical "effects" (in real or gedanken experiments) when interpreted in terms of these topological solitons. This is an encouragement for further physico-mathematical collaboration.

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Application of Altman's contractor techniques to nonlinear integral equations for Green's functions of augmented quantum field theory

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Altman's theory of contractors and contractor directions is applied to equations for connected irreducible Green's functions of Klauder's augmented quantum field theory in the ϕ^4 model, and sufficient conditions for existence of solutions are discussed.

I. INTRODUCTION

Recently, Klauder[1] proposed an alternative quantization scheme, based on a different choice of the measure $\mathcal{D}'\Phi$ used in the definition of the generating functional. The theory can be formulated in operator formalism as well as in Green's function formalism. Here, we consider the ϕ^4 model in Green's function formalism. In terms of irreducible many-point functions, the first two equations of the infinite sequence of equations read

$$\begin{aligned} &G_2(p)+\tfrac{1}{2}\int d^4k(k^2-m^2)G_4(p,-p,k,-k)\\ &\quad+2\lambda\int d^4k_1d^4k_2d^4k_3\{G_4(k_1,k_2,p,-k_1-k_2-p)\\ &\quad\times G_2^{-1}(k_1+k_2+p)G_4(k_3,-k_1-k_2-k_3,k_1+k_2+p,-p)\\ &\quad+G_4(p,-p,k_1,-k_1)G_2^{-1}(k_1)G_4(k_2,k_3,-k_1,k_1-k_2-k_3)\\ &\quad+G_6(k_1,k_2,k_3,-k_1-k_2-k_3,p,-p)\}=0 \qquad (1.1)\\ &-G_4+\tfrac{1}{4}[K^*G_4^{**2*}(G_2^{-1})]+\tfrac{1}{4}[K^*G_6]+(4)\lambda[G_4^{**3*}(G_2^{-1})]\\ &\quad+(3)\lambda[G_4^*G_6^*(G_2^{-1})]+\lambda[^*G_8]=0 \qquad (1.2)\end{aligned}$$

[for the meaning of Eq. (1.2), see Fig. 1], where the G_n $(n\geq 6)$ stand for connected irreducible (in any channel) n-point functions. The integrals in Eq. (1.1) should be interpreted as subtracted at $p^2=m^2$, i.e.,

$$\int d^4k(k^2-m^2)G_4(p,-p,k,-k)=\int_{m^2}^{p^2}d(p'^2)\frac{d}{d(p'^2)}\int d^4k\times(k^2-m^2)(p'^2-m^2)^2G_4(p',-p',k,-k)/(p^2-m^2-i\epsilon)^2, \qquad (1.3)$$

etc., in particular,

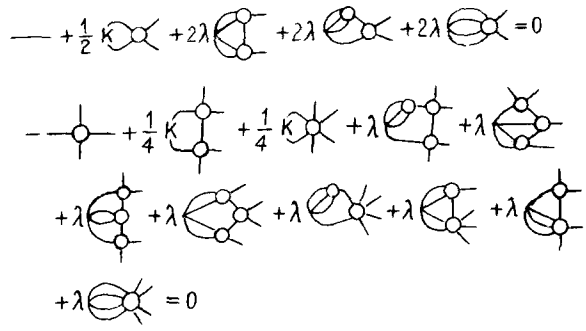

FIG. 1. Graphical representation of Eqs. (1.1), (1.2).

$$\begin{aligned}&\Big[\int d^4k_1d^4k_2d^4k_3G_4(p,-p,k_1,-k_1)G_2^{-1}(k_1)\\ &\quad\times G_4(k_2,k_3,-k_1,k_1-k_2-k_3)\Big]_{\text{ren}}\\ &\quad=\int_{m^2}^{p^2}d(p'^2)\frac{d}{d(p'^2)}\int d^4k_1G_4(p',-p',k_1,-k_1)\\ &\quad\times(p'^2-m^2)^2\int_{m^2}^{k_1^2}d(k_1'^2)\frac{d}{d(k_1'^2)}\int d^4k_2d^4k_3\\ &\quad\times G_2^{-1}(k_1')G_4(k_2,k_3,-k_1',k_1'-k_2-k_3) \qquad (1.4)\end{aligned}$$

so that every term in (1.1) has a simple pole at $p^2=m^2$. Consequently, there is no possibility of calculating "dynamically generated" mass. On the other hand, an interesting feature of Eq. (1.2) is the absence of the terms shown in Fig. 2, which appear in the Schwinger–Dyson equation for four-point function in the conventional quantization and have undesirable asymptotic behavior. Because of the absence of those terms in Eq. (1.2), one cannot perform a subtraction (renormalization) in Eq. (1.2). In other words, the integrals in Eq. (1.2) must be interpreted as they stand.

In this note, we consider the descending problem: To determine lower many-point functions when higher many-point functions are given as "boundary conditions" to the functional differential equation for the generating functional.

II. DESCENDING PROBLEM FOR THE EQUATION FOR TWO-POINT FUNCTION

In this section, we consider Eq. (1.1) when $G_4(p_1,p_2,p_3,-p_1-p_2-p_3)$ and $G_6(p_1,-p_1,p_2,p_3,p_4,-p_2-p_3-p_4)$ with desirable asymptotic behavior are specified as input.

Let us assume that $G_2(p)$ has no zeros, i.e., $G_2(p)$ has an unsubtracted spectral representation. Then one can rewrite Eq. (1.1) as follows:

$$\begin{aligned}&L(p)+((p^2-m^2)\{M(p)+(2)2\lambda[G_4^{**2*}(KL)](p)\})^{-1}\\ &\quad:=\Lambda[L](p)=0,\end{aligned} \qquad (2.1)$$

FIG. 2. Diagrams that are present in the conventional Schwinger–Dyson equation for G_4, but absent in Eq. (1.2).

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$$M(p)=\tfrac{1}{2}[K*G_4](p)+2\lambda[*G_6](p), \tag{2.2}$$

where

$$L(p):=[(p^2-m^2)G_2(p)]^{-1}. \tag{2.3}$$

Some comments are in order. If G_2 does not have a zero, $L(p)$ does not have a pole, so that one can expect nice behavior of L. On the other hand, if the two-point function G_2 has a subtracted spectral representation

$$G_2(p)=i(p^2-\mu^2)\int ds\rho(s)(p^2-s-i\epsilon)^{-1}(s-\mu^2)^{-1} \tag{2.4}$$

with asymptotic behavior $G_2(p)\big|_{p^2|\to\infty}(p^2)^0$, then the pole-free object to be looked for is

$$\mathfrak{L}(p)=(p^2-\mu^2)[(p^2-m^2)G_2(p)]^{-1} \tag{2.5}$$

and we get the following equation

$$\mathfrak{L}(p)+[\mathfrak{R}(p)\{M(p)+(2)2\lambda[G_4{}^{**2}*(\mathfrak{R}\mathfrak{L})](p)\}]^{-1}=0,$$
$$\mathfrak{R}(p)=\frac{p^2-m^2}{p^2-\mu^2}. \tag{2.6}$$

However, this equation cannot be consistent because asymptotically $\mathfrak{L}(p)\sim(p^2)^0$ while the second term on the lhs behaves asymptotically $\sim(p^2)$, which is a consequence of renormalization. If one takes recipe

$$[K*G_4]_{\rm ren}(p)=\int_{m^2}^{p^2}a(p'^2)\int_{m^2}^{p'^2}d(p''^2)\frac{d^2}{d(p''^2)^2}\int d^4k \times(k^2-m^2)(p''^2-m^2)^2G_4(p'',-p'',k,-k) \times(p^2-m^2-i\epsilon)^{-1}, \tag{2.7}$$

etc., then $G_2(p)$ cannot have a pole at $p^2=m^2$, so that such a recipe is not acceptable. This is an important difference from the descending problem in the canonical quantum field theory.[2] Therefore, Klauder's arguments[3] in favor of subtracted spectral representation do not apply to the case of $\lambda\neq 0$.

Suppose $G_4(p_1,p_2,p_3,-p_1-p_2-p_3)$ and $G_6(p_1,-p_1,p_2,p_3,p_4,-p_2-p_3-p_4)$ are so chosen that $|M(p)|\geq c_1\geq 0$. Then, an interesting feature of the nonlinear operator Λ is that it has first divided difference.

Definition 1: If a linear operator $V(L_1,L_2):\mathcal{D}(\Lambda)\times\mathcal{D}(\Lambda)\subset\mathbb{B}_2\times\mathbb{B}_2\to\mathfrak{L}(\mathbb{B}_2\to Y)$ satifies the relationship

$$V(L_1,L_2)(L_1-L_2)=\Lambda(L_1)-\Lambda(L_2) \tag{2.8}$$

V is called the first divided difference operator of the nonlinear operator Λ.

It is easy to see that the operator

$$V(L_1,L_2)=I-\frac{(2)2\lambda[G_4{}^{**2}*(K\cdot)]}{\{M+(2)2\lambda[G_4{}^{**2}*(KL_1)]\}\{M+(2)2\lambda[G_4{}^{**2}*(KL_2)]\}K} \tag{2.9}$$

satisfies the condition (2.8). So, let us try to apply Altman's theory[4] of two-point contractors.

Definition 2: A map $R: X\times X\to\mathfrak{L}(Y\to X)$ is said to be a two-point contractor for (nonlinear) operator P with majorant function Q if

$$\|P(x+R(x,\bar{x})y)-Px-y\|\leq Q(\|y\|,\|x-\bar{x}\|) \text{ for } x,\bar{x}\in X,\ y\in Y \text{ whenever } x+R(x,\bar{x})y\in D(P).$$

Lemma 1: If $\|V(L_1,L_2)^{-1}\|\leq c_2$ for some constant c_2, and

$$\|V(L_1,L_2)-V(L_3,L_4)\|<c_3(\|L_1-L_3\|+\|L_2-L_4\|) \quad \forall L_1,L_2,L_3,L_4\in\mathcal{D}(\Lambda)$$

then $W(L_1,L_2):=V(L_1,L_2)^{-1}$ is a two-point contractor. (For proof, see Altman.[4])

It is easy to check that our V satisfies the conditions of Lemma 1, if $\mathcal{D}(\Lambda)$ is restricted to be sufficiently small and/or c_1 is sufficiently large. For the theory of two-point contractors to be applicable, the nonlinear operator Λ need not be continuous, but closed. In other words, G_4 may be a distribution. So, we take the input $\{G_4(\cdots),G_6(p,-p,\cdots)\}$ and the Banach space $\mathbb{B}_2\ni L$ so that the map Λ is closed. We have the following theorem (Altman[4]).

Theorem 1: Let $\Lambda:\mathcal{D}(\Lambda)\subset\mathbb{B}_2\to Y$ be a closed nonlinear operator with $\mathcal{D}(\Lambda)\supset S(L_0,\rho)$, and L_0 and L_0' be so chosen that $\|\Lambda(L_0)\|\leq\eta$, $\|L_0-L_0'\|<\beta\eta$, $q:=2\eta c_3\beta^2<1$, $\rho:=\beta\eta t^*$, $t^*:=\sum_{n=0}^{\infty}q^{2^n-1}$. Suppose that $\|W(L,\bar{L})\|<\beta$ for $L,\bar{L}\in\mathcal{D}(\Lambda)$ and

$$\|\Lambda(L+W(L,\bar{L})J)-\Lambda(L)-J\|\leq\beta c_3(\beta\|J\|+\|L-\bar{L}\|)\|J\|$$

for $L,\bar{L}\in S$ whenever $L+W(L,\bar{L})J\in S$. Then the sequence $\{L_n\}$ defined by

$$L_{n+1}=L_n-W(L_n,\bar{L}_n)\Lambda(L_n),\quad \bar{L}_{n+1}=L_{n+1}-W(L_n,\bar{L}_n)\Lambda(L_{n+1})$$

converges to a solution L^* of the equation $\Lambda(L)=0$. All the L_n's lie in S and the rate of covergence is given by

$$\|L^*-L_n\|\leq t^*q^{2^n-1}\beta\eta.$$

Our next task is to verify that we can choose $\mathcal{D}(\Lambda)$ so that the conditions of Theorem 1 are satisfied. Of the three constants β,η,c_3, one can choose and c_3 sufficiently small so that the condition $q<1$ be satisfied, while β is always larger than 1. For c_3 to be small, it is desirable that $|M(p)(p^2-m^2)^{-1}|$ is large. In other words, for the theorem to be applicable, G_4 and/or G_6 should be large even when λ is small. This is a very strange feature of the descending problem in the augmented quantum field theory. Alternatively, one can restrict $\mathcal{D}(\Lambda)$ so that c_3 is small, if one finds a nice L_0 by luck.

III. DESCENDING PROBLEM FROM GIVEN HIGHER MANY-POINT FUNCTIONS

Next question one might ask is whether one can determine G_2 and G_4 if G_6 and G_8 are given. Becuase of complicated constraints, one cannot specify G_6 and G_8 arbitrarily. But one can pose the following problem. Suppose the function $H(p)=[*G_6(p,-p,\cdots)]$ and sum of terms in Eq. (1.2) involving G_6 or G_8, which we denote by N, are given as input with appropriate asymptotic behavior. Then the equations to be considered are

$$L(p)+(\{2\lambda HK+\tfrac{1}{2}[K*G_4]K+(2)2\lambda[G_4{}^{**2}*(KL)]\}(p))^{-1}=0, \tag{3.1}$$

$$-G_4+N+\tfrac{1}{4}[K*G_4{}^{**2}*(KL)]+(4)\lambda[G_4{}^{**3}*(KL)^{**2}]=0. \tag{3.2}$$

As $G_n(p_1,\ldots,p_n)$ has a pole when a p_i is on mass shell,

one cannot metrize the space of candidates for G_4. So, we define semiamputated many-point functions

$$\Gamma_n(p_1,\ldots,p_n)=\prod_{i=1}^{n}(p_i^2-m^2)G_n(p_1,\ldots,p_n). \tag{3.3}$$

Equations (3.1) and (3.2) are rewritten as follows:

$$L(p)+(\{2\lambda HK^2+\tfrac{1}{2}[K^{-1}*\Gamma_4]+(2)2\lambda[(K^{-1})^{**4}*\Gamma_4^{**2}*(K^{-1}L)]\}(p))^{-1}K(p)=0, \tag{3.4}$$

$$-\Gamma_4+KN+\tfrac{1}{4}[(K^{-1})^{*}\Gamma_4^{**2}*(K^{-1}L)]+(4)\lambda[(K^{-1})^{**4}*\Gamma_4^{**2}*(K^{-1}L)^{**2}]=0, \tag{3.5}$$

Now, we define the norms of semiamputated many-point functions by

$$\|\Gamma_n\|_{\mathbb{B}_n}=\alpha_{n1}\sup|\Gamma_n(p,\ldots,p_n)|+\alpha_{n2}\sup\Big|\prod_{i=1}^{n}|p_i^2|^{\xi}\Gamma_n(p_1,\ldots,p_n)\Big|,\quad \xi>1 \tag{3.6}$$

so that the Banach spaces of semiamputated many-point functions do not contain functions with undesirable asymptotic behavior. Now, one can regard Eqs. (3.4) and (3.5) as an operator equation in the direct sum of Banach spaces, $\mathbb{B}_2\oplus\mathbb{B}_4$. For one or another theorem concerning contractors to be applicable H must be large and N must be small. The former is a very odd requirement, but if one gives such H and N as input, one can apply Altman's theory of contractor directions.[4]

Definition 3: Let X be a complete metric space and Y be a real or complex Banach space. Let P be an operator $P:\mathcal{D}(P)\subset X\to Y$ and $x\in X$. Then $\mathcal{T}_x(P)=\mathcal{T}_x(P,q)$ is to be set of special contractor directions for P at $x\subset D(P)$, if there exist a positive constant $q<1$ and a function $B\subset\mathcal{B}$ such that for every $y\in\mathcal{T}_x(P)$ there exist a positive number $\epsilon=\epsilon(x,y)$ and an element $\bar{x}\in\mathcal{D}(P)$ such that

$$\|P\bar{x}-Px-\epsilon y\|\le q\epsilon\|y\|,\quad d(\bar{x}-x)\le B(\|y\|),$$

where $\mathcal{B}$ is the class of increasing continuous function $B(s)$ such that $B(s)>0$ for $s>0$ and

$$\int_0^a s^{-1}B(s)ds<\infty \quad \text{for some } a>0.$$

Theorem 2: Suppose (1) the operator $P:\mathcal{D}(P)\subset Y$ is closed on $U:=\mathcal{D}(P)\cap S(x_0,r)$; (2) for any $x\in U_0\equiv\mathcal{D}(P)\cap S(x_0,r)$, set of special contractor directions is dense in some ball in Y; (3) $r\ge(1-q)^{-1}\int_0^a s^{-1}B(s)ds$, $a=\|P(x_0)\|\exp(1-q)$. Then there exists an element $x^*\in U$ such that $P(x^*)=0$. (For proof see Altman.[4])

In application to our Eqs. (3.4) and (3.5), we take $x_0=\{L_0,\Gamma_{4(0)}\}=\{0,0\}\in X$ and define the norm

$$\|\{L,\Gamma_4\}\|_X=c_4\|L\|_{\mathbb{B}_2}+c_5\|\Gamma_4\|_{\mathbb{B}_4} \tag{3.7}$$

with appropriate c_4 and c_5. Then, the number

$$a=[c_4(2\lambda)^{-1}\|(HK)^{-1}\|+c_5\|NK^4\|]\exp(1-q) \tag{3.8}$$

and, consequently, r can be chosen sufficiently small so that the conditions of Theorem 2 be satisfied. Here, one need not assume that the range is closed.

The snag of this theorem is, however, that it does not give an algorithm for construction of an approximate solution. In order to formulate an algorithm, one has to assume Fréchet differentiability of the map involved. Let us write Eqs. (3.4), (3.5) abstractly $\Xi(L,\Gamma_4;H,N)=0$. If one restricts Banach spaces of L and Γ_4 from $\mathbb{B}_2$ and $\mathbb{B}_4$ to $\mathbb{B}_2'$ and $\mathbb{B}_4'$, respectively, so that the map Ξ is Fréchet differentiable with respect to L and Γ_4, and the Fréchet derivative $\Xi'(L',\Gamma_4';H,N;\ ,\ )$ is invertible for $\{L',\Gamma_4'\}\in\mathcal{G}$ and some other conditions are satisfied, one can apply Newton–Kantorovich type schemes, where $\mathcal{G}$ is an appropriate convex set in $\mathbb{B}_2'\oplus\mathbb{B}_4'$ (See Altman,[4] Janko,[5] Kantorovich and Akilov,[6] or Krasnosel'skiĭ *et al.*[7])

IV. RENORMALIZATION

The next problem is the renormalization of a solution of equations with a given input. In general, G_2 obtained as a solution of Eq. (1.1) or (3.4) has a residue $z\neq1$ at $p^2=m^2$, and Γ_4 obtained as solution of Eq. (3.4) does not assume the value $\Gamma(0,0,0,0)=\lambda$. Therefore, we must renormalize G_2: $G_2^r=z^{-1}G_2$. Then Eq. (1.1) is rewritten as follows:

$$G_2^r+\tfrac{1}{2}[K*G_4^r]+(2)2\lambda[G_4^{r**2}*(G_2^r)^{-1}]+2\lambda[*G_6^r]=0 \tag{4.1}$$

with $G_n^r=z^{-1}G_n$ for any $n\in\mathbb{Z}^+$. In other words, Eq. (1.1) is invariant under the renormalization. However, one cannot make Γ_4 assume the value $\Gamma_4(0,0,0,0)=\lambda$ for a given input. An interpretation is that λ in Eq. (4.1) is not the strength of interaction but a parameter. On the other hand, if one takes with $\Gamma_4(0,0,0,0)=\lambda$ and $G_2(p)$ with unit residue at $p^2=m^2$, Eq. (4.1) can be regarded as a linear constraint on $\Gamma_6(q,-q,\cdots)$.

Alternatively, if G_6(or Γ_6) and G_2 are given, Eq. (4.1) becomes a nonlinear constraint on Γ_4. Though we do not have a proof, it seems that this constraint can be satisfied by Γ_4 such that $\Gamma_4(0,0,0,0)=\lambda$. Rather there seem to be infinitely many Γ_4's that satisfy the constraint.

V. CONCLUDING REMARKS

So far we have discussed descending problems and existence theorem. On the other hand, if one begins with G_2 and Γ_4 as input and ascend the hierarchy of equations, G_6 need not be large, but there appear many linear and nonlinear constraints for G_n $(n>6)$. Though it seems that there is a continuum of sequences of functions that satisfy these conditions, we do not know how to construct (approximately) one or another sequence of these functions with proper symmetry.

On the other hand, so far as existence of solution is concerned, Fréchet differentiability may be violated in one way or another.

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Spherically symmetric static conformally flat solutions in Brans–Dicke and Sen–Dunn theories of gravitation

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Vacuum field equations for the static spherically symmetric conformally flat metric are obtained in Brans–Dicke and Sen–Dunn scalar-tensor theories of gravitation. Closed form exact solutions to the field equations are presented and studied in both the theories.

1. INTRODUCTION

Brans and Dicke[1] have formulated a scalar-tensor theory of gravitation in which the tensor field alone is geometrized and the scalar field is alien to geometry. Recently, Sen and Dunn[2] proposed a new scalar-tensor theory of gravitation in a modified Riemannian manifold in which both the scalar and tensor fields have intrinsic geometrical significance. The scalar field, in this theory, is characterized by the function $x^0 = x^0(x^i)$ where x^i are the coordinates in the four-dimensional Lyra manifold and the tensor field is identified with the metric tensor g_{ij} of the manifold.

The field equations in vacuum given by Sen and Dunn for the combined scalar and tensor fields are

$$G_{ij} = \omega(x^0)^{-2}(x^0_{,j}x^0_{,j} - \tfrac{1}{2}g_{ij}x^0_{,k}x^{0,k}), \tag{1}$$

where $\omega = \frac{3}{2}$ and G_{ij} is the usual Einstein tensor. It was pointed out that these equations are identical to the Brans—Dicke equations in vacuum, namely

$$\begin{aligned} G_{ij} &= \omega\phi^{-2}(\phi_{,i}\phi_{,j} - \tfrac{1}{2}g_{ij}\phi_{,k}\phi^{,k}) \\ &\quad + \phi^{-1}(\phi_{,i;j} - g_{ij}\Box\phi), \ \Box\phi = 0, \end{aligned} \tag{2}$$

if the scalar function satisfied the condition

$$\phi_{,i;j} - g_{ij}\Box\phi = 0$$

and $\omega = \frac{3}{2}$. However, the gravitational constant must be redefined. Brans[3] and Mahanta and Reddy[4–6] gave spherically symmetric static solutions in the Brans—Dicke theory of gravitation, while Sen and Dunn[2] and Halford[7] have obtained the same in Sen—Dunn theory. Penney[8] and Gurses[9] have obtained exact solutions for massless scalar meson fields with a conformally flat metric. Recently, Ray[10] has given a complete set of exact solutions for both massive and massless scalar mesons in a conformally flat metric. The present note is an attempt to obtain exact solutions for both Brans—Dicke and Sen—Dunn scalar-tensor fields in a static conformally flat space.

2. FIELD EQUATIONS AND SOLUTIONS

We consider the spherically symmetric conformally flat line element

$$ds^2 = e^{\alpha}(dr^2 + r^2d\vartheta^2 + r^2\sin^2\vartheta d\Phi^2 - dt^2), \tag{3}$$

where α is a function of r alone. For this space—time the nonvanishing components of the Einstein tensor are given by

$$G^1_1 = e^{-\alpha}\left(\frac{3}{4}\alpha'^2 + \frac{2\alpha'}{r}\right),$$

$$G^2_2 = G^3_3 = e^{-\alpha}\left(\alpha'' + \frac{\alpha'^2}{4} + \frac{\alpha'}{r}\right), \tag{4}$$

$$G^4_4 = e^{-\alpha}\left(\alpha'' + \frac{\alpha'^2}{4} + \frac{2\alpha'}{r}\right).$$

Here a superscript prime indicates differentiation with respect to r.

A. Brans-Dicke Theory

Taking ϕ as a function of r only and using (4) and (3) in (2), the Brans—Dicke field equations, in vacuum, can be written as

$$\begin{aligned} &\tfrac{3}{4}\alpha'^2 + \frac{2\alpha'}{r} = \frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{\phi''}{\phi} - \frac{1}{2}\alpha'\frac{\phi'}{\phi}, \\ &\alpha'' + \frac{\alpha'^2}{4} + \frac{\alpha'}{r} = -\frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{1}{2}\alpha'\frac{\phi'}{\phi} + \frac{1}{r}\frac{\phi'}{\phi}, \\ &\alpha'' + \frac{\alpha'^2}{4} + \frac{2\alpha'}{r} = -\frac{\omega}{2}\left(\frac{\phi'}{\phi}\right)^2 + \frac{1}{2}\alpha'\frac{\phi'}{\phi}, \\ &\phi'' + \phi'\left(\alpha' + \frac{1}{r}\right) = 0. \end{aligned} \tag{5}$$

It can be easily verified that when the scalar field ϕ is constant the field equations yield a solution which describes an empty flat space—time in Einstein's theory. When ϕ is not a constant, but is a function of r only, the Brans—Dicke field equations (5) admit the closed form exact solution given by

$$\alpha = c/r, \quad \phi = \phi_0 e^{-c/r},$$

with

$$\omega = -\tfrac{3}{2}, \tag{6}$$

where c and ϕ_0 are constants of integration. Thus the only spherically symmetric static conformally flat solutions of the Brans—Dicke vacuum equations are flat space—time and

$$ds^2 = e^{\alpha}(dr^2 + r^2d\vartheta^2 + r^2\sin^2\vartheta\, d\Phi^2 - dt^2)$$

with

$$e^{\alpha} = e^{c/r}, \ \phi = \phi_0 e^{-c/r}, \text{ and } \omega = -3/2. \tag{7}$$

Also it can be seen that when $r \to \infty$ the solution (6) reduces to empty flat space—time in Einstein's theory with $\phi = \phi_0$.

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B. Sen-Dunn theory

Taking the scalar field x^0 as a function of r only and using (4) and (3) in (1), the Sen—Dunn field equations, in vacuum, are

$$\tfrac{3}{4}\alpha'^2 + \frac{2\alpha'}{r} = \frac{\omega}{2}\left(\frac{x^{0\prime}}{x^0}\right)^2,$$

$$\alpha'' + \frac{\alpha'^2}{4} + \frac{\alpha'}{r} = -\frac{\omega}{2}\left(\frac{x^{0\prime}}{x^0}\right)^2, \tag{8}$$

$$\alpha'' + \frac{\alpha'^2}{4} + \frac{2\alpha'}{r} = \frac{\omega}{2}\left(\frac{x^{0\prime}}{x^0}\right)^2,$$

which admit the solution

$$ds^2 = e^{\alpha}(dr^2 + r^2 d\theta^2 + r^2 \sin^2\theta\, d\Phi^2 - dt^2) \tag{9}$$

with $\alpha = \text{constant}$ and $x^0 = \text{constant}$, which describes nothing but the flat space—time. Hence it can be said that a conformally flat static vacuum metric in Sen—Dunn theory describes simply a flat space—time.

3. CONCLUSIONS

Closed form exact solutions have been obtained for a static spherically symmetric conformally flat vacuum metric in the scalar-tensor theories formulated by Brans and Dicke and Sen and Dunn. It is observed that the only spherically symmetric static conformally flat vacuum solutions in Brans—Dicke theory are the flat space—time and the solution given by (7). It is also found that a static conformally flat vacuum metric in Sen—Dunn theory describes simply an empty flat space—time.

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Slow motion approximation in predictive relativistic mechanics. II. A noninteraction theorem for interactions derived from the classical field theory[a]

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By adopting an Aristotle invariant Lagrangian formalism (equivalent to canonically representing only this subgroup of the Poincaré group) and imposing a certain separability condition and a Newtonian limit on the Lagrangian, we obtain the most general Lagrangian up to c^{-3} order that verifies these properties and leads to a relativistic invariant dynamic (i.e., it satisfies the Currie–Hill equations). It contains up to c^{-2} order, all the Lagrangians known up to the present time. It is shown that the interactions derived from the classical field theory (CFT) do not admit approximated Lagrangians up to c^{-4} order, and thus this constitutes a noninteraction theorem for said interactions and somehow justifies some authors' attitudes of abandoning the Lagrangian formalism (dropping the canonical character of position coordinates) when they construct a Hamiltonian formalism for these systems.

1. INTRODUCTION

In the framework of predictive relativistic mechanics (PRM), an isolated system of N structureless point particles is governed by an ordinary second order differential system over $\mathbb{R}^{3N}$,

$$\frac{dx_a^i}{dt} = v_a^i, \quad \frac{dv_a^i}{dt} = \mu_a^i(x_b^j, v_c^k; t), \tag{1.1}$$

where the μ_a^i functions, which we will call accelerations, must satisfy the Currie–Hill equations[1–4]:

$$\frac{\partial \mu_a^i}{\partial t} = 0, \tag{1.2a}$$

$$\epsilon_b \frac{\partial \mu_a^i}{\partial x_b^j} = 0, \tag{1.2b}$$

$$\eta_j{}^i{}_k \left[x_b^k \frac{\partial \mu_a^i}{\partial x_b^j} + v_b^k \frac{\partial \mu_a^i}{\partial v_b^j} \right] = \eta_j{}^i{}_k \mu_a^k, \tag{1.2c}$$

$$c^{-2}(x_{aj} - x_{bj}) v_b^k \frac{\partial \mu_a^i}{\partial x_b^k} + [\epsilon_b \delta_j^k - c^{-2} v_{bj} v_b^k - c^{-2}(x_{bj} - x_{aj}) \mu_b^k] \frac{\partial \mu_a^i}{\partial v_b^k}$$
$$= -c^{-2}(2 v_{aj} \mu_a^i + v_a^i \mu_{aj}), \tag{1.2d}$$

which state the invariance of the set of trajectories by the Poincaré group. $i, j, k, \cdots = 1, 2, 3$; $a, b, c, a', \cdots = 1, 2, \ldots, N$; a' is always different from a; η_{ijk} is the Levi-Civita pseudotensor with $\eta_{123} = +1$; all indices follow the summation convention; c is the velocity of light in vacuum; $\epsilon^a = \epsilon_a = 1$.

On the other hand, the difficulty arising from a Poincaré invariant Lagrangian formalism (the canonical realization of this group on phase space) is well known for such dynamic systems because this assumption leads to the Currie, Jordan, and Sudarshan[5,6] noninteraction theorem: The unique systems which admit this Lagrangian formulation are the free particle systems ($\mu_a^i = 0$). In particular, Hill's[7] and the authors'[8] proof of this theorem make known the essential role played by two assumptions: (a) the position coordinates of the x_a^i particles are canonical, and (b) the pure Lorentz transformations act like a set of canonical transformations. First attempts to circumvent the noninteraction theorem coincide in substituting assumption (b) for another less restrictive one, because dropping assumption (a) would be equivalent to renouncing the traditional Lagrangian formalism (we , however, remark that a Hamiltonian formalism can be satisfactorily developed in which the position coordinates are *not* canonical[9–11]). Thus, for example, in Ref. 12 (resp. 13) assumption (b) is substituted for the following: the energy, the linear momentum, and the angular momentum are assumed to appropriately transform as regards pure Lorentz transformations (resp. the dynamic system is invariant by space inversion and the angular momentum is assumed to appropriately transform as regards pure Lorentz transformations). However, in both cases one arrives at the two noninteraction theorems for the two particle systems.

Moreover, the authors have recently proven[8] that the Currie, Jordan, and Sudarshan noninteraction theorem starts to be effective above the c^{-6} order. Then the most general family of approximated Lagrangians up to c^{-4} order, possessing a Newtonian limit, is obtained, although this family does not contain the approximated Lagrangians up to c^{-2} order deduced from the classical field theory (CFT).

All these facts have led to us adopt an Aristotle[14] invariant Lagrangian formalism in this paper (this is equivalent to canonically representing only this subgroup of the Poincaré group and is also equivalent to dropping assumption (b), although we impose a certain separability condition and a Newtonian limit on the Lagrangian. With the perturbation technique of c^{-1} expansions, we found the most general Lagrangian up to c^{-3} order that satisfies the previous properties. In particular, it includes up to c^{-2} order the Lagrangians obtained by means of: (i) classical fields theory, (ii) Poincaré invariant canonical formulation, [15] (iii)

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Poincaré invariant action,[16] (iv) Lagrangians postulated "ad hoc",[17] (v) Lagrangians corresponding to a single particle and a later symmetrization.[18]

Moreover, we show by using the general dynamic obtained in Ref. 19 (approximated up to c^{-4} order that satisfies the Currie–Hill equations, is invariant by space inversion and possesses a Newtonian limit) that the Lagrangians derived from the CFT cannot be extended up to c^{-4} order because of their incompatibility with the invariance equations. Thus, we obtain a noninteraction theorem for the interactions derived from the CFT.

As we believe the previous assumption (the Aristotle group is canonically represented on the phase space) to be the minimal condition we must impose in order to be able to define, without ambiguity, the conservative quantities: energy, momentum, and angular momentum of the system, we conclude that at least for certain interactions (among which are the well-known electromagnetic and gravitational interactions) only a description by means of approximated Lagrangians up to c^{-3} order is possible.

We think this result is the strongest at the moment which justifies the attitudes adopted by some authors[9–11] in dropping the Lagrangian formalism (or more exactly the canonical character of position cordinates x_a^i) and in constructing a Hamiltonian formulation for such systems.

Finally, we include an Appendix dedicated to the uniqueness of the Lagrangian up to c^{-3} order.

2. LAGRANGIAN FORMULATION INVARIANT UNDER THE ARISTOTLE GROUP, DEVELOPMENT IN c^{-1}

(A) Let us consider a dynamic system of type (1.1) which is invariant under the Aristotle group, i.e., such that it verifies Eqs. (1.2a), (1.2b), and (1.2c). As has been shown in Ref. 8, the fact that such a system admits a Lagrangian formulation compatible with its invariance is expressed by the existence of a function $L(t; x_a^i, v_b^j)$ satisfying the following conditions:

$$Q\frac{\partial L}{\partial v_a^i}=\frac{\partial L}{\partial x_a^i},\quad \det\left(\frac{\partial^2 L}{\partial v_a^i \partial v_b^j}\right)\neq 0, \tag{2.1}$$

$$\frac{\partial L}{\partial t}=0, \tag{2.2a}$$

$$\epsilon_b \frac{\partial L}{\partial x_b^j}=0, \tag{2.2b}$$

$$\eta_j{}^l{}_k\left(x_b^k\frac{\partial L}{\partial x_b^l}+v_b^k\frac{\partial L}{\partial v_b^l}\right)=0, \tag{2.2c}$$

where Q is a first order differential linear operator defined as follows,

$$Q\equiv\frac{\partial}{\partial t}+v_b^j\frac{\partial}{\partial x_b^j}+\mu_b^j(x_c^k, v_d^l)\frac{\partial}{\partial v_b^j} \tag{2.3}$$

Equations (2.1) merely state that the dynamic system (1.1) is a Lagrangian one. On the other hand, Eqs. (2.2) point out that $L(t; x_a^i, v_b^j)$ is an invariant function under space–time translations and space rotations (Aristotle group). We will also assume that L is invariant under parity.

As is well known, if the Lagrangian L admits a symmetry it is possible to automatically associate a first integral with the corresponding dynamic system. Consequently, Eqs. (2.2) permit the association of the seven first integrals with the dynamic system (1.1). Such integrals are traditionally identified with energy, linear momentum, and angular momentum. These conserved magnitudes are respectively expressed in the following way:

$$H\equiv v_a^i\frac{\partial L}{\partial v_a^i}-L, \tag{2.4a}$$

$$P_j\equiv\epsilon_b\frac{\partial L}{\partial v_b^j}, \tag{2.4b}$$

$$J_j\equiv\eta_{jk}{}^l x_a^k\frac{\partial L}{\partial v_a^l}. \tag{2.4c}$$

In this paper, we are going to limit ourselves to the consideration of a dynamic system (1.1) that contains only two particles ($N=2$). According to this hypothesis the general solution of Eqs. (2.2) will be an arbitrary function of six independent particular solutions, for example (following the notation given in Ref. 19)

$$r\equiv+(x_{aa'}^i x_{aa'i})^{1/2},\quad s\equiv\tfrac{1}{2}x_{aa'}^i v_{aa'i},$$
$$q\equiv\tfrac{1}{2}\eta_a x_{aa'}^i(v_{ai}+v_{a'i}),\quad y_a\equiv v_a^i v_{ai}\equiv v_a^2,\quad y\equiv v_{aa'}^i v_{aa'i}\equiv v^2, \tag{2.5}$$

where

$$\eta_a:\ \eta_1\equiv+1,\quad \eta_2\equiv-1;\quad x_{aa'}^i\equiv x_a^i-x_{a'}^i;\quad v_{aa'}^i\equiv v_a^i-v_{a'}^i. \tag{2.6}$$

Therefore, we will hereinafter write

$$L=L(r, s, q, y_a, y). \tag{2.7}$$

It is clear that the dynamic system associated with this Lagrangian is Aristotle and parity invariant.

(B) Next, we suppose that the Lagrangian (2.7) admits a development on a power series of c^{-1} according to the following structure,

$$L=\sum_{n=0}^{\infty}\frac{1}{c^n}L^{(n)}, \tag{2.8}$$

where the functions $L^{(n)}(r, s, q, y_a, y)$ are independent of c. In addition, we will suppose that the following conditions are verified:

$$L^{(0)}\equiv\tfrac{1}{2}\epsilon^a m_a v_a^2-V(r),$$
$$\lim_{r\to\infty}V(r)=\lim_{r\to\infty}r^{-1}\dot{V}(r)=0\quad\left(\cdot\equiv\frac{d}{dr}\right), \tag{2.9a}$$

$$L^{(2)}\equiv 0, \tag{2.9b}$$

$$\lim_{r\to\infty}L=c^2\epsilon^a m_a\left[1-\left(1-\frac{v_a^2}{c^2}\right)^{1/2}\right], \tag{2.10}$$

where $m_a>0$ is the mass of the particle a. Conditions (2.9) can be summarized by saying that the dynamic system has a "classical Newtonian limit." Let us remark that $L^{(0)}$ is the Lagrangian corresponding to a system of two particles that interact through a $V(r)$ potential. Condition (2.10) expresses the separable

character of said interaction, i.e., when the distance between both particles is infinite, the Lagrangian is reduced to the one corresponding to free particles.

Let us now assume that accelerations μ_a^i also admit a development on a power series of c^{-1} in the following way,

$$\mu_a^i = \sum_{n=0}^{\infty} \frac{1}{c^n} \mu_a^{(n)i}, \tag{2.11}$$

$\mu_a^{(n)i}$ being independent of c. By introducing developments (2.8) and (2.11) into the Lagrange equations (2.1) and taking into account expressions (2.9) for $L^{(0)}$ and $L^{(1)}$, as well as (2.2a), we can easily obtain

$$m_a \left[\mu_a^{(0)i} + \frac{1}{c}\mu_a^{(1)i} + \sum_{n=2}^{\infty} \frac{1}{c^n} \mu_a^{(n)i}\right] + \sum_{n=2}^{\infty} \frac{1}{c^n} D \frac{\partial L^{(n)}}{\partial v_i^a} + \sum_{\substack{p+s=n=3 \\ p=1,\ldots,n-2 \\ s=2,\ldots,n-1}}^{\infty} \frac{1}{c^n} Q^{(p)} \frac{\partial L^{(s)}}{\partial v_i^a} = -\frac{W}{r^2} x_{aa'}^i + \sum_{n=2}^{\infty} \frac{1}{c^n} \frac{\partial L^{(n)}}{\partial x_i^a}, \tag{2.12}$$

where the following notation has been used:

$$D \equiv v_b^k \frac{\partial}{\partial x_b^k} + \mu_b^{(0)k} \frac{\partial}{\partial v_b^k},$$

$$Q^{(p)} \equiv \mu_b^{(p)k} \frac{\partial}{\partial v_b^k} \quad (p \geq 1), \tag{2.13}$$

$$W(r) \equiv rV(r).$$

Therefore, by matching the same order terms for c^{-1} on both sides of (2.12),

$$m_a \mu_a^{(0)i} \equiv F_a^{(0)i} = -\frac{W}{r^2} x_{aa'}^i, \quad m_a \mu_a^{(1)i} \equiv F_a^{(1)i} = 0, \tag{2.14a}$$

$$(n \geq 2): \; m_a \mu_a^{(n)i} \equiv F_a^{(n)i} = \frac{\partial L^{(n)}}{\partial x_i^a} - D \frac{\partial L^{(n)}}{\partial v_i^a} - \sum_{\substack{p+s=n \\ p=1,\ldots,n-2 \\ s=2,\ldots,n-1}} Q^{(p)} \frac{\partial L^{(s)}}{\partial v_i^a} \tag{2.14b}$$

that is to say, according to hypothesis (2.9), the force is Newtonian for order zero and null for order one. On the other hand, the following conditions are met for any order up to c^{-4} inclusively,

$$F_a^{(2)i} = \Delta_a^i L^{(2)}, \tag{2.15a}$$

$$F_a^{(3)i} = \Delta_a^i L^{(3)}, \tag{2.15b}$$

$$F_a^{(4)i} = \Delta_a^i L^{(4)} - Q^{(2)} \frac{\partial L^{(2)}}{\partial v_i^a}, \tag{2.15c}$$

where the Δ_a^i differential operators are defined as

$$\Delta_a^i \equiv \frac{\partial}{\partial x_i^a} - D \frac{\partial}{\partial v_i^a}. \tag{2.16}$$

Moreover, up to the above-mentioned c^{-4} order, the limit condition (2.10) is expressed in the following way:

$$\lim_{r \to \infty} L^{(2)} = \tfrac{1}{8} \epsilon^a m_a y_a^2, \tag{2.17a}$$

$$\lim_{r \to \infty} L^{(3)} = 0, \tag{2.17b}$$

$$\lim_{r \to \infty} L^{(4)} = \tfrac{1}{16} \epsilon^a m_a y_a^3. \tag{2.17c}$$

(C) Next, let us establish a lemma that will prove most useful in later sections.

Lemma 1: The general solution of the differential system

$$G_j \Delta_a^i L = 0 \quad \left(G_j \equiv \epsilon_b \frac{\partial}{\partial v_b^j}\right), \tag{2.18}$$

that has the (2.7) dependence and satisfies the limit condition $\lim_{r \to \infty} L = 0$, has the following structure,

$$L(r, s, q, y_a, y) = \frac{\beta(r)}{r^2} sq + \frac{\alpha(r)}{4} \eta_a (y_a - y_{a'}) + f(r, s, y), \tag{2.19}$$

$\beta(r) \equiv r\dot{\alpha}(r)$, $\alpha(r)$, and $f(r, s, y)$ being arbitrary functions, such that

$$\lim_{r \to \infty} \alpha(r) = \lim_{r \to \infty} r^{-2} \beta(r) = \lim_{r \to \infty} f(r, s, y) = 0. \tag{2.20}$$

Moreover, the general solution (2.19) verifies

$$\Delta_a^i L \equiv \left\{-\frac{\eta_a \beta}{4r^2} y - \frac{\eta_a}{r}\left(\frac{\beta}{r^2}\right)' s^2 + \eta_a m_a^{-1} \frac{(\alpha+\beta) W}{2r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{2W}{\mu r^2}\frac{\partial f}{\partial y} - \frac{1}{2} D \frac{\partial f}{\partial s}\right\} x_{aa'}^i - \left\{\frac{\eta_a \beta}{r^2} s + 2D \frac{\partial f}{\partial y}\right\} v_{aa'}^i, \tag{2.21}$$

where μ is the "reduced mass" of the system, i.e.,

$$\mu \equiv \frac{m_1 m_2}{m_1 + m_2}. \tag{2.22}$$

Proof: As long as function L is assumed to be dependent on the variables (2.5), such a function is invariant under space translation, and consequently the differential system (2.18) is equivalent to the system $\Delta_a^i G_j L = 0$. In fact

$$G_j \Delta_a^i L \equiv G_j \left(\frac{\partial L}{\partial x_i^a} - D \frac{\partial L}{\partial v_i^a}\right)$$

$$= \frac{\partial}{\partial x_i^a} G_j L - D \frac{\partial}{\partial v_i^a} G_j L - \frac{\partial^2 L}{\partial x_b^l \partial v_i^a} G_j v_b^l$$

$$= \Delta_a^i G_j L - \epsilon_b \frac{\partial^2 L}{\partial x_b^j \partial v_i^a} \equiv \Delta_a^i G_j L. \tag{2.23}$$

On the other hand, a simple calculation shows that this system ($\Delta_a^i G_j L = 0$) is equivalent to the following one:

$$2D \frac{\partial L}{\partial y^a} = \eta_a \frac{\partial L}{\partial q}, \tag{2.24a}$$

$$\eta_a \frac{\partial^2 L}{\partial v_i^a \partial q} + 2D \frac{\partial^2 L}{\partial r_i^a \partial y^a} = 2 \frac{\partial^2 L}{\partial x_i^a \partial y^a}, \tag{2.24b}$$

$$-\eta_a \frac{\partial^2 L}{\partial r_i^a \partial q} + 2D \frac{\partial^2 L}{\partial r_i^a \partial y^{a'}}, \; = 2 \frac{\partial^2 L}{\partial x_i^a \partial y^{a'}}, \tag{2.24c}$$

$$\eta_a D \frac{\partial^2 L}{\partial r_i^a \partial q} - \frac{2W}{r^2}\left(m_a^{-1} \frac{\partial^2 L}{\partial r_i^a \partial y^a} - m_{a'}^{-1} \frac{\partial^2 L}{\partial r_i^a \partial y^{a'}}\right) = \eta_a \frac{\partial^2 L}{\partial x_i^a \partial q}. \tag{2.24d}$$

Taking into account (2.24a), Eqs. (2.24b) and (2.24c) can be written as follows,

$$\frac{\partial}{\partial x_i^a}\left(\epsilon_b \frac{\partial L}{\partial y_b}\right) = 0, \quad \eta_a \frac{\partial^2 L}{\partial v_i^a \partial q} = 2 \frac{\partial^2 L}{\partial x_i^a \partial y^a} \tag{2.25}$$

which, when developed, lead to the system:

$$\frac{\partial^2 L}{\partial q^2}=0,\quad \frac{\partial^2 L}{\partial q\partial y^a}=0,$$
$$\frac{\partial}{\partial u}\left(\epsilon_b\frac{\partial L}{\partial y_b}\right)=0,\quad \frac{\partial}{\partial s}\left(\epsilon_b\frac{\partial L}{\partial y_b}\right)=0,$$
$$\frac{\partial^2 L}{\partial s\partial q}=4\frac{\partial}{\partial u}\left(\frac{\partial L}{\partial y_1}-\frac{\partial L}{\partial y_2}\right),\quad 4\frac{\partial^2 L}{\partial q\partial y}=\frac{\partial}{\partial s}\left(\frac{\partial L}{\partial y_1}-\frac{\partial L}{\partial y_2}\right), \tag{2.26}$$

where $u\equiv r^2$. Equations (2.26) automatically imply that function L must have the structure

$$L=q\cdot A(u,s,y)+(y_1-y_2)\cdot B(u,s,y)+C(y,y_a)+E(u,s,y), \tag{2.27}$$

where A, B, C, and E are functions subject only to the verification of the conditions

$$\frac{\partial B}{\partial u}=\frac{1}{8}\frac{\partial A}{\partial s},\quad \frac{\partial B}{\partial s}=2\frac{\partial A}{\partial y}. \tag{2.28}$$

From (2.27) and making the change of variables $t\equiv y_1-y_2$, $z\equiv y_1+y_2$, equations (2.24a) can be written

$$D\frac{\partial C}{\partial z}=0,\quad D\left(\frac{\partial C}{\partial t}+B\right)=\tfrac{1}{2}A. \tag{2.29}$$

Likewise, Eqs. (2.24d) lead to the system:

$$m\frac{\partial C}{\partial z}-\frac{\partial C}{\partial t}=g(y),\quad m\equiv\frac{m_1-m_2}{m_1+m_2},$$
$$D\frac{\partial A}{\partial s}=\frac{4W}{\mu u}\frac{\partial A}{\partial y}+\frac{2W}{\mu u}\frac{\partial B}{\partial s}+4\frac{\partial A}{\partial u}, \tag{2.30}$$
$$D\frac{\partial A}{\partial y}=\frac{2W}{\mu u}\frac{\partial B}{\partial y}-\frac{2W}{\mu u}\frac{dg}{dy},$$

where $g(y)$ is an arbitrary function.

Next, let us show that condition $\lim_{r\to\infty}L=0$ implies that it is possible to assume $C(y,y_a)=0$ without a loss of generality. Indeed, since the said condition is assumed to be valid for any value of the (s,q,y_a,y) variables, the following limits exist according to (2.27),

$$\lim_{r\to\infty}A(u,s,y)\equiv A^*(s,y),\quad \lim_{r\to\infty}B(u,s,y)\equiv B^*(s,y),$$
$$\lim_{r\to\infty}E(u,s,y)\equiv E^*(s,y), \tag{2.31}$$

so that the following expression is verified,

$$q\cdot A^*(s,y)+(y_1-y_2)B^*(s,y)+C(y,y_a)+E^*(s,y)=0. \tag{2.32}$$

It is now clear that $A^*=0$ and that functions B^* and E^* cannot be dependent on variable s. Consequently, (2.32) gives the following structure for $C(y,y_a)$,

$$C(y,y_a)=-(y_1-y_2)B^*(y)-E^*(y) \tag{2.33}$$

and thus (2.27) can be rewritten

$$L=q\cdot A(u,s,y)+(y_1-y_2)[B(u,s,y)-B^*(y)]+E(u,s,y)-E^*(y), \tag{2.34}$$

i.e., a redefinition of functions $B(u,s,y)$ and $E(u,s,y)$ is sufficient for $C(y,y_a)=0$ to be assumed.

Summing up the previous results: Function L should have the following structure,

$$L=q\cdot A(u,s,y)+(y_1-y_2)\cdot B(u,s,y)+E(u,s,y), \tag{2.35}$$

where A, B, and E must satisfy the following equations and limit conditions

$$\frac{\partial B}{\partial u}=\frac{1}{8}\frac{\partial A}{\partial s},\quad \frac{\partial B}{\partial s}=2\frac{\partial A}{\partial y}, \tag{2.36}$$
$$DB=\tfrac{1}{2}A, \tag{2.37}$$
$$D\frac{\partial A}{\partial s}=\frac{4W}{\mu u}\frac{\partial A}{\partial y}+\frac{2W}{\mu u}\frac{\partial B}{\partial s}+4\frac{\partial A}{\partial u}, \tag{2.38}$$
$$D\frac{\partial A}{\partial y}=\frac{2W}{\mu u}\frac{\partial B}{\partial y}, \tag{2.39}$$
$$\lim_{r\to\infty}A=\lim_{r\to\infty}B=\lim_{r\to\infty}E=0. \tag{2.40}$$

Obviously, (2.39) is identically verified as a consequence of (2.36) and (2.37). On the other hand, taking into consideration (2.36), (2.37), and $\lim_{r\to\infty}V=0$, it can be concluded that (2.38) is equivalent to

$$s\frac{\partial B}{\partial y}=-\frac{u}{4}\frac{\partial A}{\partial y}. \tag{2.41}$$

From (2.36) and (2.41), (2.37) turns out to be equivalent to

$$s\frac{\partial A}{\partial s}+2y\frac{\partial A}{\partial y}=A \tag{2.42}$$

whose general solution is

$$A=s\cdot\bar{A}(u,\omega),\quad \omega\equiv\frac{4}{u}-\frac{y}{s^2}, \tag{2.43}$$

which when introduced in (2.41) determines the following structure for function B,

$$B=-\frac{u}{4}\bar{A}(u,\omega)+\bar{B}(u,s), \tag{2.44}$$

$\bar{A}$ and $\bar{B}$ being arbitrary functions.

Only equations (2.36) remain for study, using results (2.43) and (2.44). To start with, we should note that (2.36b) leads to

$$\bar{A}(u,\omega)=\Phi(u)\cdot\ln\omega+\Psi(u),$$
$$\bar{B}(u,s)=-\frac{u}{2}\Phi(u)\ln s+\delta(u), \tag{2.45}$$

where Φ, Ψ, and δ are arbitrary functions. Then (2.36a) implies

$$\Phi=0,\quad \Psi=\frac{1}{r}\dot{\alpha}(r),\quad \delta=\tfrac{1}{4}[\alpha(r)+r\dot{\alpha}(r)]+\text{const}, \tag{2.46}$$

where $\alpha(r)$ is an arbitrary function of r and $\dot{\alpha}\equiv d\alpha/dr$. By introducing these expressions in (2.43) and (2.44)

$$A=\frac{s}{r}\dot{\alpha}(r),\quad B=\tfrac{1}{4}\alpha(r)+\text{const}. \tag{2.47}$$

By including the additive constant in $\alpha(r)$ and according to (2.35),

$$L=\frac{\beta(r)}{r^2}sq+\frac{\alpha(r)}{4}(y_1-y_2)+f(r,s,y), \tag{2.48}$$

where functions $\alpha(r)$, $\beta(r)\equiv r\dot{\alpha}(r)$, and $f(r,s,y)$ must satisfy the limit conditions deduced from (2.40),

$$\lim_{r\to\infty}\alpha(r)=\lim_{r\to\infty}r^{-2}\beta(r)=\lim_{r\to\infty}f(r,s,y)=0. \tag{2.49}$$

Thus the first part of the lemma has been proved. Let us now prove equality (2.21). From (2.7):

$$\frac{\partial L}{\partial x_i^a}=\frac{1}{r}\frac{\partial L}{\partial r}x^i_{aa'}+\frac{1}{2}\frac{\partial L}{\partial s}v^i_{aa'}+\frac{1}{2}\eta_a\frac{\partial L}{\partial q}(v_a^i+v_{a'}^i),$$
$$\frac{\partial L}{\partial v_i^a}=\frac{1}{2}\left(\frac{\partial L}{\partial s}+\eta_a\frac{\partial L}{\partial q}\right)x^i_{aa'}+2\frac{\partial L}{\partial y}v^i_{aa'}+2\frac{\partial L}{\partial y^a}v_a^i, \tag{2.50}$$

and consequently, taking into account (2.13) and (2.14a)

$$D\frac{\partial L}{\partial v_i^a}=\left\{\frac{1}{2}D\left(\frac{\partial L}{\partial s}+\eta_a\frac{\partial L}{\partial q}\right)-\frac{2W}{\mu r^2}\frac{\partial L}{\partial y}-m_a^{-1}\frac{2W}{r^2}\frac{\partial L}{\partial y^a}\right\}x^i_{aa'}$$
$$+\left(\frac{1}{2}\frac{\partial L}{\partial s}+\frac{\eta_a}{2}\frac{\partial L}{\partial q}+2D\frac{\partial L}{\partial y}\right)v^i_{aa'}+2D\frac{\partial L}{\partial y^a}\cdot v_a^i \tag{2.51}$$

and remembering definition (2.16),

$$\Delta_a^iL=\left\{\frac{1}{r}\frac{\partial L}{\partial r}-\frac{1}{2}D\left(\frac{\partial L}{\partial s}\right)+\eta_a\left(\frac{\partial L}{\partial q}\right)+\frac{2W}{\mu r^2}\frac{\partial L}{\partial y}\right.$$
$$\left.+m_a^{-1}\frac{2W}{r^2}\frac{\partial L}{\partial y^a}\right\}x^i_{aa'}$$
$$-\eta_a\left(\frac{\partial L}{\partial q}+2D\frac{\partial L}{\partial y}\right)v^i_{aa'}+\left(\eta_a\frac{\partial L}{\partial q}-2D\frac{\partial L}{\partial y^a}\right)v_a^i. \tag{2.52}$$

Nevertheless, according to (2.48), one easily obtains

$$2D\frac{\partial L}{\partial y^a}=\eta_a\frac{\partial L}{\partial q}=\frac{\eta_a\beta(r)}{r^2}s,$$

$$\frac{1}{r}\frac{\partial L}{\partial r}=\frac{1}{r}\left(\frac{\beta}{r^2}\right)^{\cdot}sq+(y_1-y_2)\frac{\beta(r)}{4r^2}+\frac{1}{r}\frac{\partial f}{\partial r},$$

$$\tfrac{1}{2}D\left(\frac{\partial L}{\partial s}+\eta_a\frac{\partial L}{\partial q}\right)=\frac{\eta_a\beta(r)}{4r^2}y+\frac{\eta_a}{r}\left(\frac{\beta}{r^2}\right)^{\cdot}s(s+\eta_aq)$$

$$+(y_1-y_2)\frac{\beta(r)}{4r^2}-\eta_am_a^{-1}W\frac{\beta(r)}{4r^2}+\frac{1}{2}D\frac{\partial f}{\partial s}$$

When these results are introduced in (2.51) they automatically lead to the (2.21) equality. Q.E.D.

3. APPROXIMATE LAGRANGIAN UP TO ORDER c^{-3}

In this section, we assume that the dynamic system (1.1) is invariant under the whole Poincaré group, i.e., so that all the Eqs. (1.2) are verified. We will then try to find, up to the approximation order c^{-3}, the most general Lagrangian which is Aristotle invariant and describes a dynamic system of the mentioned type for the case of two particles. We will also impose the condition that the interaction be separable and that there be a Newtonian limit in the sense that was specified in the previous section.

Let us consider Eqs. (1.2d) [in Ref. 8 it was shown that these equations are the only ones that cannot be deduced from (2.1) and (2.2)] which state the invariance of the dynamic system under the pure Lorentz transformations. For the $N=2$ case:

$$-G_j\mu_a^i=\frac{1}{c^2}\left\{x_{aa'j}\left(v^k_{a'}\frac{\partial\mu_a^i}{\partial x^{a'k}}+\mu^k_{a'}\frac{\partial\mu_a^i}{\partial v^{a'k}}\right)\right.$$
$$\left.-v_j^bR_b\mu_a^i+2v_{aj}\mu_a^i+v_a^i\mu_{aj}\right\}, \tag{3.1}$$

where R_b is the first order linear differential operator

$$R_b\equiv v_b^k\frac{\partial}{\partial v^{bk}}. \tag{3.2}$$

By introducing (2.11) in Eqs. (3.1), for each order in c^{-1}, the following is obtained:

$$G_j\mu_a^{(0)i}=0,\quad G_j\mu_a^{(1)i}=0, \tag{3.3a}$$

$$-G_j\mu_a^{(n)i}=x_{aa'j}D_a\mu_a^{(n-2)i}-v_j^bR_b\mu_a^{(n-2)i}+2v_{aj}\mu_a^{(n-2)i}$$
$$+v_a^i\mu_{aj}^{(n-2)}+x_{aa'j}\sum_{\substack{p+s=n-2\\ p=1,\dots,n-2\\ s=0,\dots,n-3}}\mu_a^{(p)k}\frac{\partial\mu_a^{(s)i}}{\partial v^{a'k}}\quad(n>1), \tag{3.3b}$$

where the D_a operators are defined as

$$D_a\equiv v_a^k\frac{\partial}{\partial x^{ak}}+\mu_a^{(0)k}\frac{\partial}{\partial v^{ak}}. \tag{3.4}$$

Equations (3.3a) are coherent with Eqs. (2.14a). On the other hand, taking into account (2.14a), Eqs. (3.3b) are written (for the second and third orders) in the following way,

$$-G_jF_a^{(2)i}=x_{aa'j}D_aF_a^{(0)i}+2v_{aj}F_a^{(0)i}+v_a^iF_{aj}^{(0)}, \tag{3.5a}$$

$$G_jF_a^{(3)i}=0, \tag{3.5b}$$

which, along with (2.15a) and (2.15b), imply for the first and second orders of the Lagrangian, the following equations:

$$-G_j\Delta_a^iL^{(2)}=x_{aa'j}D_aF_a^{(0)i}+2v_{aj}F_a^{(0)i}+v_a^iF_{aj}^{(0)}, \tag{3.6a}$$

$$G_j\Delta_a^iL^{(3)}=0. \tag{3.6b}$$

In addition, it is necessary to take into account the limit conditions (2.17a) and (2.17b).

Let us start with order c^{-2}. Without difficulty, it can be verified that the function

$$L_p^{(2)}\equiv\tfrac{1}{8}\epsilon^am_ay_a^2-\frac{W}{2r^2}q^2+\frac{V}{4}\epsilon^ay_a \tag{3.7}$$

is a particular solution of (3.6a) and satisfies the limit condition (2.17a). Consequently, the general solution we are looking for is

$$L^{(2)}=L_p^{(2)}+L_*^{(2)}, \tag{3.8}$$

where $L_*^{(2)}$ is the general solution of the homogeneous system $G_j\Delta_a^iL_*^{(2)}=0$, which fulfills the condition $\lim_{r\to\infty}L_*^{(2)}=0$. By applying Lemma 1 and taking into account (3.7) and (3.8), one obtains for the second order,

$$L^{(2)}=\tfrac{1}{8}\epsilon^am_av_a^4-\frac{W}{2r^2}q^2+\frac{V}{4}(v_1^2+v_2^2)+\frac{\beta}{r^2}sq+\frac{\alpha}{4}(v_1^2-v_2^2)$$
$$+f(r,s,v^2), \tag{3.9}$$

where $\alpha(r)$, $\beta(r)\equiv r\dot\alpha(r)$, and $f(r,s,v^2)$ must satisfy

$$\lim_{r\to\infty}\alpha=\lim_{r\to\infty}r^{-2}\beta=\lim_{r\to\infty}f=0. \tag{3.10}$$

Let us now consider order c^{-3}. From (3.6b), (2.17b), and Lemma 1, we obtain

$$L^{(3)} = \frac{\delta}{r^2} sq + \frac{\gamma}{4}(v_1^2 - v_2^2) + g(r, s, v^2), \tag{3.11}$$

where $\gamma(r)$, $\delta(r) \equiv r\dot{\gamma}(r)$, and $g(r, s, v^2)$ must satisfy

$$\lim_{r\to\infty}\gamma = \lim_{r\to\infty} r^{-2}\delta = \lim_{r\to\infty} g = 0. \tag{3.12}$$

In summing up, up to order c^{-3}, the most general Aristotle invariant Lagranigan having a Newtonian limit, is separable and provides relativistic invariant trajectories, is given by

$$L = \tfrac{1}{2}\epsilon^a m_a v_a^2 - V + \frac{1}{c^2}\left\{\tfrac{1}{8}\epsilon^a m_a v_a^4 - \frac{W}{2r^2} q^2 + \frac{V}{4}(v_1^2 + v_2^2) + \frac{\beta}{r^2} sq + \frac{\alpha}{4}(v_1^2 - v_2^2) + f\right\} + \frac{1}{c^3}\left\{\frac{\delta}{r^2} sq + \frac{\gamma}{4}(v_1^2 - v_2^2) + g\right\}, \tag{3.13}$$

where $V(r)$, $W(r) \equiv r\dot{V}(r)$, $\alpha(r)$, $\beta(r) \equiv r\dot{\alpha}(r)$, $f(r, s, v^2)$, $\gamma(r)$, $\delta(r) \equiv r\dot{\gamma}(r)$, and $g(r, s, v^2)$ must satisfy the limit conditions (2.9a), (3.10), and (3.12).

Let us remark that up to order c^{-2}, Lagrangian (3.13) coincides with the one we obtained in Ref. 8, which by hypothesis was developed for much more severe invariance conditions. In addition, one should note that the "forces" deduced from Lagrangian (3.13) [by means of (2.15), (2.16) and (2.21)] have the same structure as those which we worked out in Ref. 19.

4. THE STANDARD LAGRANGIANS UP TO c^{-2}

Lagrangian (3.13) obtained in the previous section contains (up to the c^{-2} order and as particular cases) a whole series of Lagrangians worked out by different authors in many different ways. In this section, we are going to review all of them (note that they do not ever surpass order c^{-2}) briefly indicating the different frameworks used in order to obtain each of them and their localization in the (3.13) Lagrangian.

(A) Firstly, we should point out the Lagrangians obtained (in one way or another) from the classical field theory, i.e., the scalar field, vectorial field (in particular, the electromagnetic field), and tensorial field theories (gravitational field theory within the context of general relativity). All these Lagrangians have the (3.13) structure, with the following expression for functions $\alpha(r)$ and $f(r, s, v^2)$,

$$\alpha(r) \equiv 0, \quad f(r, s, v^2) \equiv \rho \cdot V^2 - \frac{V}{4}(2l^2 - 1)v^2 + \frac{W}{2r^2} s^2, \tag{4.1}$$

where ρ and l are constants which we will specify for each case.

[A.1] *Scalar field*: When the interaction is described by means of a scalar field, two different theories have been worked out characterized by a single parameter γ that can take one or zero as values.[20,21] For the case of $\gamma = 1$, the best known Lagrangian is the Bopp Lagrangian[22] whose original derivation is rather confusing and corresponds to the following values of the constants,

$$l = \rho = 0. \tag{4.2}$$

The Lagrangian obtained in Ref. 11 is contained in the Bopp Lagrangian, corresponding to a Yukawa potential, i.e., the $V(r)$ potential is of the Yukawa type,

$$V(r) \equiv -k\frac{\exp(-\lambda r)}{r}, \tag{4.3}$$

k being the coupling constant and λ the range parameter. When $\gamma = 0$, we have found a Lagrangian only when the particle masses are identical ($m_1 = m_2$); this Lagrangian is obtained by

$$l = 0, \quad \rho = -\frac{1}{2m_1} \equiv -\frac{1}{2m_2}. \tag{4.4}$$

Likewise, we have shown that if $m_1 \neq m_2$, it is not possible to write a Lagrangian.

[A.2] *Vectorial field*: If the interaction is described by a vectorial field, it is possible to point out the Bagge Lagrangian,[23] as being especially important. As in the case of the Bopp Lagrangian, it was originally worked out in a rather confusing manner. Now the constant values are

$$l = 1, \quad \rho = 0. \tag{4.5}$$

The Darwin Lagrangian[24] constitutes a particular case of this, for it describes the electromagnetic interaction, i.e., the $V(r)$ potential is given by

$$V(r) \equiv \frac{e_1 e_2}{r}, \tag{4.6}$$

where e_a represent the electric charges of the particles. It should be pointed out that the Darwin Lagrangian was the first to be chronologically obtained.

[A.3] *Tensorial field*: The best known classical interaction described by a tensorial field is the one that corresponds to the general relativity theory. Within this context, one can place the Einstein, Infeld, and Hoffmann Lagrangian[25] which describes the gravitational interaction and which corresponds to

$$l = 2, \quad \rho = -\frac{1}{2\mu}, \quad V(r) = -G\frac{m_1 m_2}{r}, \tag{4.7}$$

G being the universal gravitational constant.

[A.4] By using the Einstein, Infeld, and Hoffmann technique, it is possible to obtain a Lagrangian which includes the gravitational and electromagnetic interactions. This Lagrangian was developed by Bazanski[26] and is a particular case of (4.1),

$$l = \left[\frac{4Gm_1m_2 - e_1e_2}{Gm_1m_2 - e_1e_2}\right]^{1/2},$$
$$\rho = \frac{(2e_1e_2 - Gm_1m_2)(m_1 + m_2) - m_1e_2^2 - m_2e_1^2}{2(e_1e_2 - Gm_1m_2)^2} G, \tag{4.8}$$
$$V(r) = \frac{e_1e_2 - Gm_1m_2}{r}.$$

As was expected, the Einstein, Infeld, and Hoffmann Lagrangian is obtained for $e_a = 0$.

[A.5] Finally, it should be pointed out that the Stabrook Lagrangian[27] is also contained in (4.1). It was obtained in order to describe the gravitational interaction between two particles, starting from the Brans–Dicke theory, in which a scalar and a tensorial

field are mixed. This Lagrangian is determined as follows:

$$l=2\left[\frac{2\omega+3}{2\omega+4}\right]^{1/2},\quad \rho=-\frac{1}{2\mu},\quad V(r)=-G\frac{m_1m_2}{r},\tag{4.9}$$

where ω is the so-called "Brans–Dicke parameter." Let us note that when $\omega\to\infty$, the Einstein, Infeld, and Hoffmann Lagrangian is obtained. Hereinafter, we will call all the approximate Lagrangians of the subsection, Lagrangians derived from the CFT.

(B) A second family of approximate Lagrangians up to the c^{-2} order having the (3.13) structure was developed by Kennedy.[18] Its derivation is based essentially on a certain symmetrization of Lagrangians corresponding to a single particle. This family adopts the following form:

$V(r)\equiv k\Phi(r)$ (k: coupling constant),

$$\alpha(r)\equiv 0,\quad f(r,s,v^2)\equiv -k\frac{\Phi}{4}(2l^2-1)v^2+k\frac{\dot{\Phi}}{2r}s^2.\tag{4.10}$$

Let us point out that these Lagrangians cannot reproduce those of type (A) for which $\rho\neq 0$, i.e., basically those which are nonlinear as regards the coupling constant.

(C) Another family of Lagrangians contained in (3.13) is the Mas[17] family, which is postulated "ad hoc" taking into account certain symmetries, in order that it lead to relativistic invariant trajectories. This family can be written as follows,

$$\alpha(r)\equiv 0,\quad f(r,s,v^2)\equiv \rho V^2-AVv^2+B\frac{W}{r^2}s^2,\tag{4.11}$$

where A, B, and ρ are arbitrary constants. The dimensions of ρ are the inverse of mass. It obviously includes Lagrangians of type (A) and (B).

(D) A fourth set of Lagrangians which are integrated in (3.13) was obtained by Woodcock and Havas.[16] Its construction is based on the existence of a Poincaré invariant action (generalization of the Fokker action). These Lagrangians are determined as follows,

$$f(r,s,v^2)\equiv A(r)v^2+B(r)s^2,\tag{4.12}$$

where $A(r)$ and $B(r)$ are arbitrary functions of its argument. It is clear that it includes some of the previously considered Lagrangians.

(E) Finally, we should mention the family of Stachel–Havas Lagrangians.[15] To obtain this family, the Poincaré group must act as a canonical transformation group (in an approximate way) upon the phase space. In addition, dimensional type requirements are imposed, as well as the necessity for the theory to have a Newtonian limit. Actually, these authors do not demand condition (1.2d) because the remaining hypotheses imply that such a condition is automatically fulfilled up to order c^{-2}. This family of Lagrangians has the following form,

$$f(r,s,v^2)\equiv v^2\sum_{l=0}^{\infty}A_l(r)B_l(z),\quad z\equiv\frac{r^2v^2}{s^2},\tag{4.13}$$

where A_l and B_l are a set of arbitrary functions.

The common feature that characterizes all the approximate Lagrangians of this section is that they provide relativistic invariant trajectories. Of these Lagrangians, the most general which has been obtained up to now, is the Stachel–Havas one [let us note that if an additive term of type $F(r)$ is included in (4.13), it will contain all the remaining ones], which in turn is a subclass of the (3.13) Lagrangian that we have obtained. We must point out, however, that in Ref. 14, a Hamiltonian whose corresponding Lagrangian is completely equivalent to (3.39) already exists, before imposing the dimensional type requirements previously mentioned [see Eq. (A17) of said reference].

On the other hand, it is worthwhile to underline the possible asymmetry (particle 1 – particle 2) which can be shown by means of the $\alpha(r)$ function and/or the $f(r,s,v^2)$ one, as well as the level of arbitrariness of the Lagrangian, due to the fact that these functions do not depend in general upon the $V(r)$ potential.

Finally, we will underscore the fact that (3.13) Lagrangian also includes some of the theories contained in the so-called PPN formalism, which corresponds to the interaction of two pointlike particles. It is also interesting to note that the (3.13) Lagrangian contains the Pauri and Prosperi[28] Lagrangian, which is obtained by means of a variational principle.

5. c^{-4} ORDER ANALYSIS

Let us once more assume the hypothesis established in the third section, i.e., let us suppose that the (1.1) dynamic system is invariant under the Poincaré group, that the interaction is separable and that a Newtonian limit exists. We are now going to study the possibility of finding, up to the c^{-4} approximation order, an Aristotle invariant Lagrangian which describes such a dynamic system for the case of two particles, i.e., the possibility of extending the Lagrangian (3.13) up to the c^{-4} order.

Let us first consider the result of Ref. 19, according to which the "forces" of this dynamic system are given (up to the c^{-4} approximation order) by the following expression,

$$\begin{aligned}F_a^i\equiv m_a\mu_a^i=&-\frac{W}{r}x^i_{aa'}+\frac{1}{c^2}\left\{\left[\frac{W}{r^2}v_a^2+\frac{1}{2r}\left(\frac{W}{r^2}\right)'\eta_aq(2s-\eta_aq)\right.\right.\\&+\frac{W}{4r^2}(2m_a^{-1}V-m_a^{-1}W+m_{a'}^{-1}W)+a_a^{(2)*}\Big]x^i_{aa'}\\&\left.+\left(\frac{W}{r^2}\eta_aq+b_a^{(2)*}\right)v^i_{aa'}\right\}+\frac{1}{c^3}\{a_a^{(3)*}x^i_{aa'}+b_a^{(3)*}v^i_{aa'}\}\\&+\frac{1}{c^4}\{(a_{pa}^{(4)}+a_a^{(4)*})x^i_{aa'}+(b_{pa}^{(4)}+b_a^{(4)*})v^i_{aa'}\}+O\left(\frac{1}{c^5}\right),\end{aligned}\tag{5.1}$$

where $a_a^{(n)*}(r,s,y)$ and $b_a^{(n)*}(r,s,y)$ are arbitrary functions. $a_{pa}^{(4)}$ and $b_{pa}^{(4)}$ are given in the mentioned reference by the following formulas:

$$a_{pa}^{(4)}\equiv\frac{1}{4r}\left(\frac{W}{r^2}\right)'(s^2+2q^2-3\eta_asq)(y_a-y_{a'})$$

$$
\begin{aligned}
&- y_a\left[\left(\frac{W}{4r^2}\right)\left(\frac{2V-W}{m_a}+\frac{W}{m_{a'}}\right)+a_a^{(2)*}\right]+\tfrac{1}{4}\epsilon^b(s+\eta_b q)\\
&\times y_b\,\frac{\partial a^{(2)*}}{\partial s}\\
&+\tfrac{1}{4}[(y_1-y_2)^2+2v^2(y_1+y_2)]\,\frac{\partial a_a^{(2)*}}{\partial y}\\
&+\frac{W}{m_{a'}r^2}\,\eta_a q\left(\frac{W}{2r^2}\,\eta_a q+b_a^{(2)*}\right)-\frac{1}{8r}\,\eta_a q(2s-\eta_a q)\\
&+\left[\frac{W}{r^2}\left(\frac{2V-W}{m_a}+\frac{W}{m_{a'}}\right)\right]^{\cdot}-\frac{1}{8r}\left[\frac{1}{r}\left(\frac{W}{r^2}\right)^{\cdot}\right]^{\cdot}\\
&\times q^2(4s^2+q^2-4\eta_a sq)-\frac{W}{2m_{a'}r}\left(\frac{W}{r^2}\right)^{\cdot}\eta_a q(s-\eta_a q)\\
&-\frac{1}{2r}\,\eta_a q(2s-\eta_a q)\,\frac{\partial a_a^{(2)*}}{\partial r}+\frac{W}{2m_{a'}r^2}\,\eta_a q\left(r^2\,\frac{\partial a_a^{(2)*}}{\partial s}\right.\\
&\left.+8s\,\frac{\partial a_a^{(2)*}}{\partial y}\right)-\frac{v^2}{4r}\,\eta_a q\left[s\left(\frac{W}{r^2}\right)^{\cdot}+r\,\frac{\partial a_a^{(2)*}}{\partial s}\right],
\end{aligned}
\tag{5.2a}
$$

$$
\begin{aligned}
{}_{p}b_a^{(4)} \equiv{}& \frac{W}{4r^2}(s-3\eta_a q)(y_a-y_{a'})-\tfrac{1}{2}b_a^{(2)*}(2y_a-y_{a'})\\
&+\tfrac{1}{4}\epsilon^b(s+\eta_b q)\,y_b\,\frac{\partial b_a^{(2)*}}{\partial s}+\tfrac{1}{4}[(y_1-y_2)^2+2v^2(y_1+y_2)]\\
&\times\frac{\partial b_a^{(2)*}}{\partial y}-\frac{1}{2r}\left(\frac{W}{r^2}\right)^{\cdot}q^2(2s-\eta_a q)-\frac{W}{4r^2}\,\eta_a q\\
&\times\left(v^2+\frac{2V-W}{m_a}+\frac{3W}{m_{a'}}\right)-\eta_a q\left[a_a^{(2)*}+\tfrac{1}{4}\left(v^2-\frac{2W}{m_{a'}}\right)\frac{\partial b_a^{(2)*}}{\partial s}\right.\\
&\left.-\frac{4W}{m_{a'}r^2}\,s\,\frac{\partial b_a^{(2)*}}{\partial y}\right]-\frac{1}{2r}\,\eta_a q(2s-\eta_a q)\,\frac{\partial b_a^{(2)*}}{\partial r}.
\end{aligned}
\tag{5.2b}
$$

On the other hand, taking into account the general expression of L (up to the c^{-3} order) and those established in (2.15a), (2.15b) for $F_a^{(2)i}$ and $F_a^{(3)i}$, one easily obtains

$$
\begin{aligned}
a_a^{(2)*} \equiv{}& -\frac{\eta_a\beta}{4r^2}v^2-\frac{\eta_a}{r}\left(\frac{\beta}{r^2}\right)^{\cdot}s^2+\frac{\eta_a W(\alpha+\beta)}{2m_a r^2}\\
&+\frac{1}{r}\,\frac{\partial f}{\partial r}+\frac{2W}{\mu r^2}\,\frac{\partial f}{\partial y}-\frac{1}{2}\,D\,\frac{\partial f}{\partial s},
\end{aligned}
\tag{5.3a}
$$

$$
b_a^{(2)*} \equiv -\frac{\eta_a\beta}{r^2}\,s-2D\,\frac{\partial f}{\partial y}. \tag{5.3b}
$$

$a_a^{(3)*}$ and $b_a^{(3)*}$ are obtained by substituting α and β for γ and δ in expressions $a_a^{(2)*}$ and $b_a^{(2)*}$, respectively.

In addition, from (2.13), (3.9), (5.1), and (5.3), we get

$$
Q^{(2)}\,\frac{\partial L^{(2)}}{\partial v_i^a}=F_a x_{aa'}^i+G_a v_{aa'}^i+Z_a v_a^i, \tag{5.4}
$$

where

$$
\begin{aligned}
F_a \equiv{}& \tfrac{1}{2}\,(m_a y_a+V+\eta_a\alpha)\,m_a^{-1}a_a^{(2)}-\frac{W}{2}(m_a^{-1}a_a^{(2)}-m_{a'}^{-1}a_{a'}^{(2)})\\
&+\eta_a\beta m_a^{-1}a_a^{(2)}-\frac{W}{r^2}\,s(m_a^{-1}b_a^{(2)}-m_{a'}^{-1}b_{a'}^{(2)})+\frac{2\eta_a\beta}{r^2}\,sm_a^{-1}b_a^{(2)}\\
&+\left(4\,\frac{\partial f}{\partial y}+\frac{r^2}{2}\,\frac{\partial^2 f}{\partial s^2}+4s\,\frac{\partial^2 f}{\partial s\,\partial y}\right)(\epsilon^b m_b^{-1}a_b^{(2)})\\
&+\left(s\,\frac{\partial^2 f}{\partial s^2}+2v^2\,\frac{\partial^2 f}{\partial s\,\partial y}\right)(\epsilon^b m_b^{-1}b_b^{(2)})\Big\},
\end{aligned}
\tag{5.5a}
$$

$$
\begin{aligned}
G_a \equiv{}& \tfrac{1}{2}\Big\{(m_a y_a+V+\eta_a\alpha)\,m_a^{-1}b_a^{(2)}+2\left(r^2\,\frac{\partial^2 f}{\partial s\,\partial y}+8s\,\frac{\partial^2 f}{\partial y^2}\right)\\
&\times(\epsilon^b m_b^{-1}a_b^{(2)})+4\left(\frac{\partial f}{\partial y}+s\,\frac{\partial^2 f}{\partial s\,\partial y}+2v^2\,\frac{\partial^2 f}{\partial y^2}\right)(\epsilon^b m_b^{-1}b_b^{(2)})\Big\},
\end{aligned}
\tag{5.5b}
$$

$$
Z_a \equiv (s+\eta_a q)\,a_a^{(2)}+\tfrac{1}{2}(v^2+y_a-y_{a'})\,b_a^{(2)}, \tag{5.5c}
$$

with

$$
a_a^{(2)} \equiv \frac{W}{r^2}\,v_a^2+\frac{1}{2r}\left(\frac{W}{r^2}\right)^{\cdot}\eta_a q(2s-\eta_a q)+\frac{W}{4r^2}\left(\frac{2V-W}{m_a}\right)+a_a^{(2)*}, \tag{5.6a}
$$

$$
b_a^{(2)} \equiv \frac{W}{r^2}\,\eta_a q+b_a^{(2)*}. \tag{5.6b}
$$

From (5.1), (5.4), and (2.15c), we obtain

$$
\Delta_a^i L^{(4)}=({}_{p}a_a^{(4)}+a_a^{(4)*}+F_a)\,x_{aa'}^i+({}_{p}b_a^{(4)}+b_a^{(4)*}+G_a)\,v_{aa'}^i+Z_a v_a^i. \tag{5.7}
$$

But $L^{(4)}$ depends only on (r, s, q, y_a, y) and consequently

$$
\begin{aligned}
\Delta_a^i L^{(4)} \equiv{}& x_{aa'}^i\left\{\frac{2}{r}\,\frac{\partial L^{(4)}}{\partial r}-\frac{1}{2}\left(\frac{\partial DL^{(4)}}{\partial s}+\eta_a\,\frac{\partial DL^{(4)}}{\partial q}\right)\right\}\\
&+v_a^i\left\{\frac{\partial L^{(4)}}{\partial s}+\eta_a\,\frac{\partial L^{(4)}}{\partial y}-2\,\frac{\partial DL^{(4)}}{\partial y}-2\,\frac{\partial DL^{(4)}}{\partial y^a}\right\}\\
&-v_{a'}^i\left\{\frac{\partial L^{(4)}}{\partial s}-\eta_a\,\frac{\partial L^{(4)}}{\partial q}-2\,\frac{\partial L^{(4)}}{\partial y}\right\}.
\end{aligned}
\tag{5.8}
$$

Then (5.7) and (5.8) lead to the following differential system on $L^{(4)}$:

$$
\eta_a\,\frac{\partial L^{(4)}}{\partial q}=-\tfrac{1}{2}({}_{p}b_a^{(4)}+b_a^{(4)*}-{}_{p}b_{a'}^{(4)}-b_{a'}^{(4)*}+G_a-G_{a'}), \tag{5.9a}
$$

$$
\eta_a\,\frac{\partial DL^{(4)}}{\partial q}=-({}_{p}a_a^{(4)}+a_a^{(4)*}-{}_{p}a_{a'}^{(4)}-a_{a'}^{(4)*}+F_a-F_{a'}), \tag{5.9b}
$$

$$
\frac{\partial DL^{(4)}}{\partial y^a}=-\tfrac{1}{2}({}_{p}b_a^{(4)}+b_a^{(4)*}-{}_{p}b_{a'}^{(4)}-b_{a'}^{(4)*}+G_a-G_{a'}+Z_a), \tag{5.9c}
$$

$$
\frac{\partial DL^{(4)}}{\partial y}-\frac{1}{2}\,\frac{\partial L^{(4)}}{\partial s}=-\tfrac{1}{4}\epsilon^b({}_{p}b_b^{(4)}+b_b^{(4)*}+G_b), \tag{5.9d}
$$

$$
\frac{\partial DL^{(4)}}{\partial s}-\frac{4}{r}\,\frac{\partial L^{(4)}}{\partial r}=-\epsilon^b({}_{p}a_b^{(4)}+a_b^{(4)*}+F_b). \tag{5.9e}
$$

Let us remark that taking into account (5.9a), Eq. (5.9b) can be written

$$
\begin{aligned}
&\frac{2W}{r^2}\left(m_a^{-1}\,\frac{\partial L^{(4)}}{\partial y^a}-m_{a'}^{-1}\,\frac{\partial L^{(4)}}{\partial y^{a'}}\right)\\
&={}_{p}a_a^{(4)}+a_a^{(4)*}-{}_{p}a_{a'}^{(4)}-a_{a'}^{(4)*}+F_a-F_{a'}\\
&\quad-\tfrac{1}{2}D({}_{p}b_a^{(4)}+b_a^{(4)*}-{}_{p}b_{a'}^{(4)}-b_{a'}^{(4)*}+G_a-G_{a'}).
\end{aligned}
\tag{5.9b'}
$$

Two of the integrability conditions of this differential system are

$$\left[\frac{\partial}{\partial y^a}-\frac{\partial}{\partial y^{a'}}\right](a_p^{(4)}+a_a^{(4)*}-a_p^{(4)}-a_{a'}^{(4)*}+F_a-F_{a'})$$
$$=\eta_a\frac{\partial}{\partial q}(b_p^{(4)}+b_a^{(4)*}-b_p^{(4)}-b_{a'}^{(4)*}+G_a-G_{a'})$$
$$+\frac{\eta_a}{2}\frac{\partial}{\partial q}(Z_a-Z_{a'}), \tag{5.10a}$$

$$4\frac{\partial}{\partial y}(a_p^{(4)}+a_a^{(4)*}-a_p^{(4)}-a_{a'}^{(4)*}+F_a-F_{a'})$$
$$=\frac{\partial}{\partial s}(b_p^{(4)}+b_a^{(4)*}-b_p^{(4)}-b_{a'}^{(4)*}+G_a-G_{a'})$$
$$+\eta_a\frac{\partial}{\partial q}\epsilon^b(b_p^{(4)}+b_b^{(4)*}+G_b). \tag{5.10b}$$

These conditions, when developed, lead respectively to the following partial differential equations over the function $f(r, s, y)$ (a function that was arbitrary at order 2 in the Lagrangian, with the exception of $\lim_{r\to\infty} f=0$),

$$\left(y-\frac{W}{\mu}\right)\frac{\partial}{\partial s}\left[D\left(\frac{\partial f}{\partial y}\right)\right]+\frac{4s}{r}\frac{\partial}{\partial r}\left[D\left(\frac{\partial f}{\partial y}\right)\right]$$
$$-\frac{8W}{\mu r^2}s\frac{\partial}{\partial y}\left[D\left(\frac{\partial f}{\partial y}\right)\right]=0, \tag{5.11a}$$

$$\frac{8}{r}\frac{\partial^2 f}{\partial r\,\partial y}-\frac{\partial^2 f}{\partial s^2}=\frac{W}{r^2}. \tag{5.11b}$$

One can then easily verify that function f, given by (4.1) (this function includes the Lagrangian derived from the CFT), does not satisfy conditions (5.11a), (5.11b). So we conclude that Lagrangians derived from CFT cannot be extended to the c^{-4} order.

We might then ask if there is some interaction that could be represented by an approximate Lagrangian up to c^{-4} order. The answer is given in Ref. 18 where the most general approximate (up to c^{-4} order) Lagrangian family, having a Newtonian limit, was obtained. This family was worked out by imposing invariance under the Poincaré group, which is obviously more restrictive than the Aristotle group used in this paper.

In summing up, we believe that it is not possible to extend the Lagrangians derived from the CFT (which are the approximate Lagrangians, up to c^{-2} order, that the classical fields theory furnish) up to the c^{-4} order, in order to get relativistic invariant trajectories.

In our opinion, this result somehow justifies some authors' attitudes when they follow a Hamiltonian approach in order to describe isolated systems, where the position coordinates are not canonical, since the Lagrangian formulation seems to be rather incompatible with the minimal symmetry corresponding to systems existing in nature.

APPENDIX

Let us consider the approximate (up to c^{-3} order) Lagrangian given by (3.13), that can be briefly written

$$L=\epsilon^a\frac{m_a v_a^2}{2}-V+\frac{1}{c^2}L^{(2)}(\alpha,f)+\frac{1}{c^3}L^{(3)}(\gamma,g)+O(c^{-4}), \tag{A1}$$

where $V(r)$, $\alpha(r)$, $\gamma(r)$, $f(r, s, v^2)$, and $g(r, s, v^2)$ are specific functions which satisfy the limit conditions (2.9a), (3.10), and (3.12),

$$\lim_{r\to\infty}V=\lim_{r\to\infty}r^{-1}\dot{V}=\lim_{r\to\infty}\alpha=\lim_{r\to\infty}r^{-1}\dot{\alpha}=\lim_{r\to\infty}\gamma$$
$$=\lim_{r\to\infty}r^{-1}\dot{\gamma}=\lim_{r\to\infty}f=\lim_{r\to\infty}g=0. \tag{A2}$$

Let $\bar{L}$ be another Lagrangian with the same structure as L, i.e.,

$$\bar{L}=\epsilon^a\frac{m_a v_a^2}{2}-\bar{V}+\frac{1}{c^2}L^{(2)}(\bar{\alpha},\bar{f})+\frac{1}{c^3}L^{(3)}(\bar{\gamma},\bar{g})+O(c^{-4}),$$

where $\bar{V}(r)$, $\bar{\alpha}(r)$, $\bar{\gamma}(r)$, $\bar{f}(r, s, v^2)$, and $\bar{g}(r, s, v^2)$ are specific functions which satisfy limit conditions similar to those expressed in (A2).

By definition, L and $\bar{L}$ are said to be equivalent if they lead to the same dynamics. Taking into account (5.1) and (5.3), L and $\bar{L}$ are equivalent if:

Order 0

$$W=\bar{W}\Rightarrow V-\bar{V}=\text{const}$$

and taking into account the (A2) limit condition for V and $\bar{V}$, we conclude that $V=\bar{V}$.

Order 2

Taking into account the result corresponding to the zero order

$$a_a^{(2)*}=\bar{a}_a^{(2)*}, \tag{A3a}$$
$$b_a^{(2)*}=\bar{b}_a^{(2)*}. \tag{A3b}$$

Obviously, (A3b) is equivalent to

$$\bar{\beta}=\beta\Rightarrow\bar{\alpha}=\alpha=\text{const},\quad D\left(\frac{\partial\bar{f}}{\partial y}-\frac{\partial f}{\partial y}\right)=0, \tag{A4a}$$

and as in the zero order, we can conclude [from (A2)] that $\bar{\alpha}=\alpha$.

Then (A3a) is equivalent to

$$D\left(\frac{\partial\bar{f}}{\partial s}-\frac{\partial f}{\partial s}\right)=\frac{2}{r}\left(\frac{\partial\bar{f}}{\partial r}-\frac{\partial f}{\partial r}\right)+\frac{4W}{\mu r^2}\left(\frac{\partial\bar{f}}{\partial y}-\frac{\partial f}{\partial y}\right). \tag{A4b}$$

Order 3

Without difficulty, one can show that $\bar{g}$ and g must satisfy equation (A4). In addition, $\bar{\gamma}=\gamma$ must be verified.

In summary, given a Lagrangian

$$L=\epsilon^b\frac{m_a v_a^2}{2}-V+\frac{1}{c^2}L^{(2)}(\alpha,f)+\frac{1}{c^3}L^{(3)}(\gamma,g)+O(c^{-4}),$$

the Lagrangian

$$\bar{L}=\epsilon^a\frac{m_a v_a^2}{2}-V+\frac{1}{c^2}L^{(2)}(\alpha,f+F)+\frac{1}{c^3}L^{(3)}(\gamma,g+G)+O(c^{-4})$$

leads to the same dynamics as the previous one (L), if and only if F and $G(r, s, v^2)$ are the general solution of the differential system

$$D\frac{\partial F}{\partial y}=0, \tag{A5a}$$

$$D\frac{\partial F}{\partial s}=\frac{2}{r}\frac{\partial F}{\partial r}+\frac{4W}{\mu r^2}\frac{\partial F}{\partial y}, \tag{A5b}$$

satisfying the limit condition [derived from (A2)]

$$\lim_{r\to\infty} F = 0. \tag{A5c}$$

Up to the moment, condition (2.10) has been imposed on the Lagrangian as the separability condition. Nevertheless, from now on, we are going to also assume the following

$$\lim_{r\to\infty} \frac{\partial L}{\partial y} = 0, \tag{A6}$$

that in relation of f and g, is expressed as

$$\lim_{r\to\infty} \frac{\partial f}{\partial y} = \lim_{r\to\infty} \frac{\partial g}{\partial y} = 0. \tag{A7}$$

so therefore, the general solution to (A5) must also verify

$$\lim_{r\to\infty} \frac{\partial F}{\partial y} = 0. \tag{A8}$$

On the other hand, it is obvious that operator D admits the following two first integrals

$$E = \tfrac{1}{2}\mu v^2 + V(r), \quad l^2 = \mu^2(r^2v^2 - 4s^2),$$

and consequently, from (A5a)

$$\frac{\partial F}{\partial y} = R(E, l^2), \tag{A9}$$

where R is an arbitrary function. Nevertheless, taking into account the (A8) limit condition, we can conclude that $R \equiv 0$, since

$$0 = \lim_{r\to\infty} \frac{\partial F}{\partial y} = \lim_{r\to\infty} R(E, l^2),$$

i.e., $F(r, s)$ does not depend on v^2.

Equation (A5b) can then be reduced to

$$\frac{2}{r}\, s\, \frac{\partial^2 F}{\partial r\, \partial s} + \frac{1}{2}\left(v^2 - \frac{W}{\mu}\right)\frac{\partial^2 F}{\partial s^2} = \frac{2}{r}\,\frac{\partial F}{\partial r}\,, \tag{A10}$$

where the action of the D operator on variables r and s has been taken into account. From (A10)

$$F = A(r)\, s + \text{const.}$$

The constant can be assumed to be zero by means of the (A5c) limit condition.

In summing up,

$$F = A(r)\, s \equiv \frac{d}{dt} B(r),$$

i.e., the Lagrangian, up to c^{-3} order, is unique with the exception of the above-mentioned total derivative.

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Group theory of the interacting Boson model of the nucleus

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Recently Arima and Iachello proposed an interacting boson model of the nucleus involving six bosons, five in a d and one in an s state. The most general interaction in this model can then be expressed in terms of Casimir operators of the following chains of subgroups of the fundamental group U(6):

$U(6) \supset U(5) \supset O(5) \supset O(3) \supset O(2)$,

$U(6) \supset O(6) \supset O(5) \supset O(3) \supset O(2)$,

$U(6) \supset SU(3) \supset O(3) \supset O(2)$.

To determine the matrix elements of this interaction in, for example, a basis characterized by the irreducible representations of the first chain of groups, then we only need to evaluate the matrix elements of the Casimir operators of O(6) and SU(3) in this basis as the others are already diagonal in it. Using results of a previous publication for the basis associated with $U(5) \supset O(5) \supset O(3)$, we obtain the matrix elements of the Casimir operators of O(6) and SU(3). Furthermore, we obtain explicitly the transformation brackets between states characterized by irreducible representations of the first two chains of groups. Numerical programs are being developed for these matrix elements from the relevant reduced $3j$ symbols for the $O(5) \supset O(3)$ chain of groups that were programmed previously.

1. INTRODUCTION

In recent work[1-3] we gave an explicit and complete determination of the states characterized by irreducible representations of the $U(5) \supset O(5) \supset O(3)$ chain of groups. The matrix elements involving these states were also obtained in terms of reduced $3j$ symbols in the $O(5) \supset O(3)$ chain of groups. These results were important in developing the group theory behind the collective model of the nucleus introduced by Bohr and Mottelson,[4] as well as for the work on transitional nuclei of Greiner and his collaborators.[5]

Simultaneously to the above papers Arima and Iachello[6] became interested in the $U(5) \supset O(5) \supset O(3)$ chain in relation with an interacting boson model that they applied to problems of nuclear structure. Later they extended this model[7] by considering the above chain as a subgroup of U(6) when to the d-boson creation operators η_m ($m = 2, 1, 0, -1, -2$) they added an s operator $\bar{\eta}$. The states for the chain

$$U(6) \supset U(5) \supset O(5) \supset O(3) \tag{1.1}$$

can be obtained by a trivial extension of those mentioned in the previous paragraph and thus explicit calculations in the interacting boson model can be carried out with the help of the reduced $3j$ symbols mentioned above.

In subsequent development of their work Arima and Iachello[8] became interested in other subgroups of the U(6) group, specifically

$$U(6) \supset O(6) \supset O(5) \supset O(3) \tag{1.2}$$

and

$$U(6) \supset SU(3) \supset O(3), \tag{1.3}$$

and in the states associated with them. Obviously the latter can be developed in terms of those characterized by the chain (1.1) if we can determine the appropriate transformation brackets that take us from them to the states characterized by the chains (1.2) or (1.3).

The object of this paper is twofold. The first one is to give explicitly the transformation brackets relating states of the chain (1.1) and (1.2) and to determine the matrix of the Casimir operator of SU(3) in the basis (1.1), whose diagonalization provides the transformation brackets between the chain (1.1) and (1.3). The second is to show that the most general interaction in a model containing d and s bosons, can be expressed in terms of the Casimir operators of the groups in the chains (1.1), (1.2), and (1.3). Thus, if we take, for example, states characterized by the irreducible representations of the chain (1.1) and obtain explicitly the matrix elements with respect to these states of the Casimir operators of O(6) and SU(3), we have also the matrix elements of an arbitrary Hamiltonian in the interacting boson model. Thus one can say that the objective of this paper is to develop the group theory of the interacting boson model.

The present analysis is of interest for other problems besides those appearing in the work of Arima and Iachello. For example, in a microscopic theory of collective motions developed by Vanagas,[9] the chains (1.1), (1.2), and (1.3) appear and thus the transformation brackets mentioned above would also be useful.

In the next section we proceed to derive the generators and Casimir operators of the groups in our different chains in terms of creation and annihilation operators associated with d and s states. In Sec. 3 we briefly summarize the results developed for the chain $U(5) \supset O(5) \supset O(3)$ and then generalize them when we consider the chain as a subgroup of U(6). In Sec. 4 we discuss the chain (1.2) and specifically the matrix elements of the Casimir operator of O(6), in the basis characterized by the chain (1.1), to obtain finally the transformation brackets relating this basis with the one characterized by the chain (1.2). In Sec. 5 we turn our attention to the Casimir operator of SU(3) and its matrix elements in the basis characterized by the chain (1.1). Finally, in the concluding section, we indicate how the most general interaction involving d and s bosons can be expressed in terms of the Casimir operators of the

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groups in the chains (1.1), (1.2), and (1.3) and briefly discuss the programs being developed for determining the matrix elements of this interaction in the basis (1.1).

2. GENERATORS AND CASIMIR OPERATORS FOR THE RELEVANT GROUPS

We shall start by giving the notation required in our discussion. As the U(5) group is related with d-states[1] we associated with it the coordinates

$$\alpha_m, \quad m=2,1,0,-1,-2, \quad \alpha^m=(-)^m\alpha_{-m}, \tag{2.1a}$$

which correspond to a Racah tensor for $l=2$. When we extend the problem to U(6) we need an extra coordinate associated with an s state which we designate by

$$\bar{\alpha} \tag{2.1b}$$

It will be useful on occasions to denote these coordinates by a single symbol

$$\alpha_{lm}, \quad l=0,2, \quad \alpha_{2m}\equiv\alpha_m, \quad \alpha_{00}\equiv\bar{\alpha} \tag{2.2}$$

and we shall use either the notation (2.1) or (2.2) depending on which proves more convenient.

The momenta associated with these coordinates will be designated by

$$\pi_{lm}=\frac{1}{i}\frac{\partial}{\partial\alpha^{lm}}, \quad l=0,2, \tag{2.3}$$

and the corresponding creation and annihilation operators are defined by

$$\eta_{lm}=\frac{1}{\sqrt{2}}(\alpha_{lm}-i\pi_{lm}), \quad \xi^{lm}=\frac{1}{\sqrt{2}}(\alpha^{lm}+i\pi^{lm}), \tag{2.4}$$

where

$$[\xi^{l'm'},\eta_{lm}]=\delta_l^{l'}\delta_m^{m'}. \tag{2.5}$$

Again we shall use, when convenient, the notation

$$\pi_{2m}\equiv\pi_m, \quad \pi_{00}\equiv\bar{\pi}, \quad \eta_{2m}\equiv\eta_m, \quad \eta_{00}\equiv\bar{\eta}, \quad \xi_{2m}\equiv\xi_m, \quad \xi_{00}\equiv\bar{\xi}. \tag{2.6}$$

We can now ask about the generators of the group U(6) and its subgroups. The former are[10]

$$C_{lm}^{l'm'}\equiv\eta_{lm}\xi^{l'm'}, \quad l,l'=0,2, \tag{2.7}$$

of which we have 36 and whose commutation relation[10] is from (2.5) given by

$$[C_{lm}^{l'm'},C_{l''m''}^{l'''m'''}]=C_{lm}^{l'''m'''}\delta_{l''}^{l'}\delta_{m''}^{m'}-C_{l''m''}^{l'm'}\delta_{l}^{l'''}\delta_{m}^{m'''}. \tag{2.8}$$

The generators of the subgroup U(5) of U(6) are obviously

$$C_{2m}^{2m'}=\eta_m\xi^{m'} \tag{2.9}$$

where we used the notation (2.6).

As is well known[1,2,10] the generators of the O(6) group will be given by the antisymmetric part of (2.7), i.e.,

$$\Lambda_{lm,l'm'}\equiv\eta_{lm}\xi_{l'm'}-\eta_{l'm'}\xi_{lm}, \tag{2.10}$$

of which we have fifteen, and ten of these,

$$\Lambda_{2m,2m'}=\eta_m\xi_{m'}-\eta_{m'}\xi_m, \tag{2.11}$$

are also the generator of O(5).

In turn, as discussed in Refs. 1 and 10 the generators of O(3) are given by

$$L_\tau=\sqrt{6}\sum_{mm'}\langle 21m\tau|2m'\rangle\eta_{m'}\xi^m$$

$$=\sqrt{5/2}\sum_{mm'}\langle 22mm'|1\tau\rangle(\eta_m\xi_{m'}-\eta_{m'}\xi_m), \quad \tau=1,0,-1, \tag{2.12}$$

which shows that this group is not only a subgroup of U(5) but also of O(5).

There remains the determination of the generators of the group SU(3) in the chain (1.3). The procedure of determining them from the generators of U(6) was extensively discussed many years ago[10,11,12] in the pioneering works on SU(3) in the shell model for the $2s-1d$ shell. From these works we see that besides L_τ the generators of SU(3) include a Racah tensor of order 2 defined by

$$Q_m\equiv-\sqrt{8\pi/15}\sum_{l'm'}\sum_{l''m''}\langle 2l'm'|r^2Y_{2m}(\theta,\varphi)|2l''m''\rangle\eta_{l'm'}\xi^{l''m''}$$

$$=\sqrt{7/3}\,[\boldsymbol{\eta}\times\boldsymbol{\xi}]_m^2+\sqrt{4/3}\,(\bar{\eta}\xi_m+\eta_m\bar{\xi}), \quad m=2,1,0,-1,-2, \tag{2.13}$$

where the kets $|2lm\rangle$ are harmonic oscillator states[13] of two quanta with the angular momentum and projection indicated. In the right-hand side of (2.13) we used the notation (2.6) and the bracket expression

$$[\boldsymbol{\eta}\times\boldsymbol{\xi}]_m^2\equiv\sum_{m'm''}\langle 22m'm''|2m\rangle\eta_{m'}\xi_{m''}, \tag{2.14}$$

together with the explicit form of the matrix element of $r^2Y_{2m}(\theta,\varphi)$ with respect to the states $|2lm\rangle$.

Having obtained the generators of all the groups in the chains (1.1), (1.2), and (1.3) we are now in a position to determine explicitly their Casimir operators. The first order ones for U(6) and U(5) are obviously

$$\hat{N}\equiv\sum_{lm}\eta_{lm}\xi^{lm}, \quad l=0,2 \tag{2.15a}$$

$$\hat{\mathcal{N}}=\sum_m\eta_m\xi^m, \tag{2.15b}$$

i.e., the corresponding number operators which commute respectively with all the generators (2.7) and (2.9). As we shall only be interested in the single row, i.e., symmetric representations of U(6), we need only the first order Casimir operators of the unitary groups.

The Casimir operator of the O(5) group, as discussed in Ref. 1, is given by

$$\Lambda^2\equiv\tfrac{1}{2}\sum_{mm'}\Lambda_{2m,2m'}\Lambda^{2m',2m}$$

$$=\hat{\mathcal{N}}(\hat{\mathcal{N}}+3)-\Big(\sum_{m'}\eta_{m'}\eta^{m'}\Big)\Big(\sum_m\xi_m\xi^m\Big), \tag{2.16}$$

and with its help we can write the Casimir operator of the O(6) group as

$$L^2\equiv\tfrac{1}{2}\sum_{lm}\sum_{l'm'}\Lambda_{lm,l'm'}\Lambda^{l'm',lm}$$

$$=\Lambda^2+K^2, \tag{2.17}$$

where

$$K^2 = \hat{N}(\bar{\eta}\bar{\xi}+1) + (\hat{N}+5)\,\bar{\eta}\bar{\xi} - \left(\sum_m \eta_m \eta^m\right)\bar{\xi}^2 - \left(\sum_m \xi_m \xi^m\right)\bar{\eta}^2. \tag{2.18}$$

We shall make extensive use of these expressions when discussing the states in the U(6) ⊃ O(6) ⊃ O(5) ⊃ O(3) chain of groups.

The Casimir operator of O(3) is of course

$$L^2 = \sum_\tau (-)^\tau L_\tau L_{-\tau}, \tag{2.19}$$

and with its help as well as with that of the operator

$$Q^2 \equiv \sum_{m=-2}^{2} (-)^m Q_m Q_{-m}, \tag{2.20}$$

the second order Casimir operator G of U(3) takes the form

$$G = Q^2 + \tfrac{1}{2}L^2 + \tfrac{4}{3}\hat{N}^2, \tag{2.21}$$

as shown in Eq. (6.39) of Ref. 10. Clearly then for eigenstates of the chain U(6) ⊃ U(5) ⊃ O(5) ⊃ O(3) in which $\hat{N}$ and L^2 are diagonal it will be enough to find the matrix of Q^2 in this basis and diagonalize it to get the eigenstates of G, which up to the ambiguities discussed at the end of Sec. 5 are characterized by irreducible representations of SU(3).

Having determined all relevant Casimir operators, we turn our attention to the basis associated with the (1.1) chain of groups.

3. THE CHAIN U(6) ⊃ U(5) ⊃ O(5) ⊃ O(3)

We start by briefly reviewing the states characterized by the irreducible representations of the U(5) ⊃ O(5) ⊃ O(3) chain of groups that were discussed in Refs. 1 and 2. These states can be denoted by the kets $|\nu\lambda s LM\rangle$ that are eigenkets of the following operators:

$$\hat{N}\,|\nu\lambda s LM\rangle = \nu\,|\nu\lambda s LM\rangle, \tag{3.1a}$$

$$\Lambda^2\,|\nu\lambda s LM\rangle = \lambda(\lambda+3)\,|\nu\lambda s LM\rangle, \tag{3.1b}$$

$$L^2\,|\nu\lambda s LM\rangle = L(L+1)\,|\nu\lambda s LM\rangle, \tag{3.1c}$$

$$L_3\,|\nu\lambda s LM\rangle = M\,|\nu\lambda s LM\rangle. \tag{3.1d}$$

There may be $d(\lambda, L)$ independent representations[1-3] L of O(3) contained in a given representation λ of O(5) and we introduce the index

$$s = 1, 2, \ldots, d(\lambda, L), \tag{3.2}$$

to distinguish them.

To obtain the explicit expression of these eigenstates it is convenient to go from the coordinates α_m, associated with quadrupole vibrations,[1,2] to those in a system fixed in the body that are related to them by

$$\alpha_m = \sum_{m'} D^{2*}_{mm'}(\vartheta_i)\, a_{m'}, \tag{3.3a}$$

where

$$a_2 = a_{-2} = (1/\sqrt{2})\,\beta\sin\gamma, \quad a_1 = a_{-1} = 0, \quad a_0 = \beta\cos\gamma, \tag{3.3b}$$

and $D^L_{mm'}(\vartheta_i)$ are Wigner functions of the Euler angles.[14] In terms of the coordinates

$$\beta,\ \gamma,\ \vartheta_1,\ \vartheta_2,\ \vartheta_3, \tag{3.4}$$

the eigenstates (3.1) take the form

$$|\nu\lambda s LM\rangle = F^\lambda_j(\beta)\,\chi^\lambda_{sLM}(\gamma, \vartheta_i), \tag{3.5}$$

$$\chi^\lambda_{sLM}(\gamma, \vartheta_i) = \pi^{5/4} 2^{-\lambda/2} \sum_K \phi^{\lambda\mu L}_K(\gamma)\, D^{L*}_{MK}(\vartheta_i). \tag{3.6}$$

In (3.5) $j = (\nu - \lambda)/2$ and

$$F^\lambda_j(\beta) = \left[\frac{2(j!)}{\Gamma(j+\lambda+\frac{5}{2})}\right]^{1/2} \beta^\lambda L_j^{\lambda+3/2}(\beta^2)\exp(-\beta^2/2), \tag{3.7}$$

with $L_j^{\lambda+3/2}$ being Laguerre polynomials.[15] The $\chi^\lambda_{sLM}(\gamma, \vartheta_i)$ play the same role for the O(5) ⊃ O(3) ⊃ O(2) chain of groups as the spherical harmonics $Y_{lm}(\theta, \varphi)$ for O(3) ⊃ O(2). They are given in (3.6) in terms of a Wigner function[14] of the Euler angles and a function $\phi^{\lambda\mu L}_K(\gamma)$ whose explicit expression appears in formulas (3.24) and (7.2) of Ref. 2. The index μ is a nonnegative integer restricted by the inequalities

$$\lambda - L \leq 3\mu \leq \lambda - (L/2) \qquad \text{if } L \text{ is even}, \tag{3.8a}$$

$$\lambda - L \leq 3\mu \leq \lambda - \left(\frac{L+3}{2}\right) \qquad \text{if } L \text{ is odd}. \tag{3.8b}$$

For a fixed λ, L the relations (3.8) indicate that if there are values of μ that satisfy them they will take all integer values between a minimum one μ_0 and a maximum one $\bar{\mu}_0 \geq \mu_0$. The index s appearing in the ket (3.1) and the angular function (3.6) is then defined as[3]

$$s = \mu - \mu_0 + 1, \tag{3.9}$$

and it takes the values (3.2) where $d(\lambda, L) = \bar{\mu}_0 - \mu_0 + 1$.

It is important to note that the angular functions (3.6) while complete are not orthonormal, as the index s is not associated with the eigenvalue of an Hermitian operator. However, we can deal with matrix elements involving the $\chi^\lambda_{sLM}(\gamma, \vartheta_i)$ either by introducing their dual[3] or by orthonormalization of the basis by the usual procedures.

So far we have the basis for the

$$\begin{array}{ccccccc} \mathrm{U}(5) & \supset & \mathrm{O}(5) & \supset & \mathrm{O}(3) & \supset & \mathrm{O}(2) \\ \nu & & \lambda & & L & & M \end{array} \tag{3.10}$$

chain of groups where underneath each one of them we have indicated the index that characterizes its irreducible representation. To include this chain as a subgroup of U(6) we write the Casimir operator (2.15a) of the latter group as

$$\hat{N} = \hat{\mathcal{N}} + \bar{\eta}\bar{\xi}. \tag{3.11}$$

The eigenstates of the number operator $\bar{\eta}\bar{\xi}$, i.e.,

$$\bar{\eta}\bar{\xi}\,|\bar{\alpha}\rangle\,|n\rangle = n\,|\bar{\alpha}\rangle\,|n\rangle \tag{3.12}$$

are obviously the wavefunctions of a one-dimensional harmonic oscillator. Thus if we define

$$\langle\alpha_m, \bar{\alpha}\,|n\nu\lambda s LM\rangle \equiv \langle\alpha_m\,|\nu\lambda s LM\rangle\,|\bar{\alpha}\,|n\rangle, \tag{3.13}$$

it is an eigenstate of (3.1) and of

$$\hat{N}\,|n\nu\lambda s LM\rangle = N\,|n\nu\lambda s LM\rangle, \tag{3.14}$$

where $N = n + \nu$.

We have obtained a complete, though nonorthonormal, set of states characterized by the irreducible representations of the chain of groups in (1.1). In the next sections we proceed to determine the states characterized by the chains (1.2) and (1.3) in terms of the kets (3.13).

4. THE CHAIN U(6) ⊃ O(6) ⊃ O(5) ⊃ O(3)

The states (3.13) are characterized by the irreducible representations of all the groups in the chain indicated in the title except for O(6). Thus if we calculate the matrix of the Casimir operator (2.17) of O(6) in the basis (3.13) we can, from its diagonalization, get linear combinations of these states characterized by the irreducible representation of O(6). We shall first carry out the calculation of this matrix and later give a closed formula for the transformation brackets between eigenstates in the chain (1.1) and (1.2).

We start by noting that from (2.16), (2.17), and (2.18) we have that

$$\mathcal{L}^2 = \hat{N}(\hat{N}+4) - \left(\sum_m \eta_m \eta^m + \bar{\eta}^2\right)\left(\sum_m \xi_m \xi^m + \bar{\xi}^2\right) \tag{4.1}$$

Thus the eigenstates satisfying[1,2]

$$\hat{N}\Psi = \rho\Psi, \quad \left(\sum_m \xi_m \xi^m + \bar{\xi}^2\right)\Psi = 0, \tag{4.2a}$$

are automatically eigenstates of $\mathcal{L}^2$ with eigenvalues $\rho(\rho+4)$, i.e.,

$$\mathcal{L}^2\Psi = \rho(\rho+4)\Psi, \quad \rho \text{ nonnegative integer}, \tag{4.2b}$$

We now apply $\mathcal{L}^2$ to the basis (3.13) and get from (2.17), (2.18), and (3.1) that

$$\mathcal{L}^2 |n\nu\lambda s L M\rangle = [\lambda(\lambda+3) + K^2]\,|n\nu\lambda s L M\rangle\,. \tag{4.3}$$

We note from the definition (2.18) of K^2 that this operator is an invariant of O(5) and thus will not affect the angular part $\chi^{\lambda}_{sLM}(\gamma, \vartheta_i)$ appearing in the state (3.13).

From the definitions (2.4) we see that K^2 takes the form

$$K^2 = \hat{\mathcal{N}}(\bar{\eta}\bar{\xi}+1) + (\hat{\mathcal{N}}+5)\,\bar{\eta}\bar{\xi} - \left(\beta^2 - \beta\frac{\partial}{\partial\beta} - \hat{\mathcal{N}} - 5\right)\bar{\xi}^2 - \left(\beta^2 + \beta\frac{\partial}{\partial\beta} - \hat{\mathcal{N}}\right)\bar{\eta}^2\,, \tag{4.4}$$

where

$$\beta^2 = \sum_m \alpha_m \alpha^m, \quad \beta\frac{\partial}{\partial\beta} = i\sum_m \alpha_m \pi^m, \tag{4.5a}$$

$$\hat{\mathcal{N}} = \tfrac{1}{2}(\beta^2 + \pi^2) - \tfrac{5}{2},$$

$$\pi^2 = \sum_m \pi_m \pi^m = -\left(\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} - \frac{\Lambda^2}{\beta^2}\right)\,. \tag{4.5b}$$

Furthermore we have for the one dimensional-oscillator $\langle\bar{\alpha}|n\rangle$ of (3.12) the following relations,

$$\bar{\eta}|n\rangle = \sqrt{n+1}\,|n+1\rangle, \quad \bar{\xi}|n\rangle = \sqrt{n}\,|n-1\rangle, \tag{4.6}$$

while for $F^{\lambda}_j(\beta)$ of (3.7) we obtain from the properties of Laguerre polynomials[15] that

$$\left(\beta^2 + \beta\frac{\partial}{\partial\beta}\right)F^{\lambda}_j(\beta) = (\lambda+2j)\,F^{\lambda}_j(\beta) - 2\sqrt{j(\lambda+j+\tfrac{3}{2})}\,F^{\lambda}_{j-1}(\beta), \tag{4.7a}$$

$$\left(\beta^2 - \beta\frac{\partial}{\partial\beta}\right)F^{\lambda}_j(\beta) = (\lambda+2j+5)\,F^{\lambda}_j(\beta) - 2[(j+1)(\lambda+j+5/2)]^{1/2}F^{\lambda}_{j+1}(\beta). \tag{4.7b}$$

Remembering now that $j = (\nu-\lambda)/2$, $n+\nu = n+2j+\lambda = N$, we can denote the states (3.13) as

$$|N-2j-\lambda, 2j+\lambda, \lambda, s, L, M\rangle, \tag{4.8}$$

and the application of the operator $\mathcal{L}^2$ to them leads from (4.3)—(4.7) to the relations

$$\mathcal{L}^2|N-2j-\lambda, 2j+\lambda, \lambda s L M\rangle = \sum_{j'} A^{N\lambda}_{jj'}\,|N-2j'-\lambda, 2j'+\lambda, \lambda s L M\rangle, \tag{4.9}$$

where $A^{N\lambda}_{jj'}$ has the selection rule $j' = j\pm 1, j$ and

$$A^{N\lambda}_{jj} = [(2j+\lambda)(2N-2\lambda-4j+1) + 5(N-\lambda-2j)] + \lambda(\lambda+3) \tag{4.10a}$$

$$A^{N\lambda}_{j,j+1} = 2[(N-\lambda-2j)(N-\lambda-2j-1)(j+1)(\lambda+j+5/2)]^{1/2} \tag{4.10b}$$

$$A^{N\lambda}_{j,j} = 2[(N-\lambda-2j+1)(N-\lambda-2j+2)\,j(\lambda+j+3/2)]^{1/2}\,. \tag{4.10c}$$

Thus the orthogonal matrix that diagonalizes $\|A^{\lambda n}_{jj'}\|$, $0 \le j, j' \le (N-\lambda)/2$, leads to the transformation brackets between the states characterized by the chains (1.1) and (1.2). The eigenvalues of the matrix $\|A^{\lambda N}_{jj'}\|$ must be of the form $\rho(\rho+4)$ with $\lambda \le \rho \le N$.

We now turn to the problem of obtaining in closed form the transformation brackets mentioned in the previous paragraph. This implies the explicit determination of the states characterized by irreducible representations of the chain of groups (1.2). To find these states rather than use the coordinates

$$\bar{\alpha}, \quad \beta, \quad \gamma, \quad \vartheta_1, \quad \vartheta_2, \quad \vartheta_3 \tag{4.11}$$

of Sec. 3, we consider new ones

$$b, \quad \delta, \quad \gamma, \quad \vartheta_1, \quad \vartheta_2, \quad \vartheta_3, \tag{4.12}$$

where

$$\bar{\alpha} = b\cos\delta, \quad \beta = b\sin\delta. \tag{4.13}$$

In terms of the variables (4.12) we see that the number operator $\hat{N}$ of (2.15a), which is associated with an harmonic oscillator of six dimensions, takes the form

$$\hat{N} = \frac{1}{2}\left(-\frac{1}{b^5}\frac{\partial}{\partial b}b^5\frac{\partial}{\partial b} + \frac{1}{b^2}\mathcal{L}^2 + b^2\right) - 3, \tag{4.14}$$

while the Casimir operator $\mathcal{L}^2$ of O(6) takes from (2.4), (2.17), (4.5), and (4.13), the form

$$\mathcal{L}^2 = \Lambda^2 - \beta^2\frac{\partial^2}{\partial\bar{\alpha}^2} - \left(\frac{1}{\beta^4}\frac{\partial}{\partial\beta}\beta^4\frac{\partial}{\partial\beta} - \frac{1}{\beta^2}\Lambda^2\right)\bar{\alpha}^2 + \left(\beta\frac{\partial}{\partial\beta} + 5\right)\bar{\alpha}\frac{\partial}{\partial\bar{\alpha}} + \beta\frac{\partial}{\partial\beta}\left(\bar{\alpha}\frac{\partial}{\partial\bar{\alpha}} + 1\right)$$

$$= -\frac{\partial^2}{\partial\delta^2} - 4\cot\delta\frac{\partial}{\partial\delta} + \frac{1}{\sin^2\delta}\Lambda^2\,. \tag{4.15}$$

Clearly an eigenstate of the operators $\hat{N}$, $\mathcal{L}^2$, Λ^2, L^2, L_3 can then be written in the form

$$|N\rho\lambda sLM\rangle = B_{N\rho\lambda} f_J^\rho(b)\, g_\lambda^\rho(\delta)\, \chi_{sLM}^\lambda(\gamma, \vartheta_i), \tag{4.16}$$

where $\chi_{sLM}^\lambda(\gamma, \vartheta_i)$ is given by (3.6), $B_{N\rho\lambda}$ is a normalization coefficient while $g_\lambda^\rho(\delta)$ satisfies the equation

$$\left(-\frac{d^2}{d\delta^2} - 4\cot\delta\,\frac{d}{d\delta} + \frac{\lambda(\lambda+3)}{\sin^2\delta}\right) g_\lambda^\rho(\delta) = \rho(\rho+4)\, g_\lambda^\rho(\delta), \tag{4.17}$$

and $f_J^\rho(b)$ in turn is determined by the equation

$$\left[\frac{1}{2}\left(-\frac{1}{b^5}\frac{d}{db}\, b^5\, \frac{d}{db} + \frac{\rho(\rho+4)}{b^2} + b^2\right) - 3\right] f_J^\rho(b) = N f_J^\rho(b), \tag{4.18}$$

where $J = (N-\rho)/2$.

From (4.17) we see that, up to a constant factor, $g_\lambda^\rho(\delta)$ is given by[15]

$$g_\lambda^\rho(\delta) = (\sin\delta)^\lambda\, C_{\rho-\lambda}^{\lambda+2}(\cos\delta), \tag{4.19}$$

where C is a Gegenbauer polynomial[15] of the indices indicated.[15] In turn, from (4.18) we obtain

$$f_J^\rho(b) = b^\rho L_J^{\rho+2}(b^2)\exp(-b^2/2), \tag{4.20}$$

where L is a Laguerre polynomial.[15]

The normalization coefficient $B_{N\rho\lambda}$ appearing in (4.16) is discussed in Appendix A, and then in Appendix B we expand the states (4.16) in terms of the states (3.13). Clearly the transformation brackets do not depend on the indices sLM as both chains have the groups $O(5) \supset O(3) \supset O(2)$ in common and thus we can denote them as

$$\begin{aligned}\langle n\nu\lambda | N\rho\lambda\rangle &= (-)^{(N-\rho+\nu-\lambda)/2}\left[\frac{2^{\rho-\lambda}(\rho+1)!\,(\rho+2)!}{2^{N-\rho}((N+\rho)/2+2)!\,(\rho-\lambda)}\right.\\ &\left.\times\frac{(\nu+\lambda+3)!\,n!\,((N-\rho)/2)!}{(\rho+\lambda+3)!\,((\nu+\lambda)/2+1)!\,((\nu-\lambda)/2)!}\right]^{1/2}\\ &\cdot\sum_s \frac{((N-\rho)/2+1)_s((\lambda-\rho)/2)_s((\lambda-\rho+1)/2)_s}{s!\,((N-\rho-\nu+\lambda)/2+s)!\,(-\rho-1)_s},\end{aligned} \tag{4.21}$$

where $n = N-\nu$ and $(a)_s$ is the Pochhamer symbol,[15] $(a)_s = a(a+1)\cdots(a+s-1)$.

The explicit form of the transformation brackets relating the chains (1.1) and (1.2) is then available.

5. THE CHAIN U(6) ⊃ SU(3) ⊃ O(3) ⊃ O(2)

As indicated at the end of Sec. 2, to obtain the states characterized by the irreducible representations of the chain of groups appearing in the title of this section, we require only the diagonalization of the matrix of the operator Q^2 defined by (2.20). For this in turn we need the matrix in the basis (3.13) of the operator Q_M of (2.13) which, from (2.2), (2.6), can also be written as

$$Q_M = \sqrt{7/12}\,\{[\alpha\times\alpha]_M^2 + [\pi\times\pi]_M^2\} + \sqrt{4/3}\,(\alpha_M\bar{\alpha} + \pi_M\bar{\pi}),$$
$$M = 2, 1, 0, -1, -2. \tag{5.1}$$

We note though that the states (3.13) are not orthonormal and thus matrix elements of $Q^2 = \sum_M (-)^M Q_M Q_{-M}$ with respect to them cannot be obtained by introducing an intermediate state of this type between Q_M and Q_{-M} and summing on the relevant quantum numbers. Rather we proceed to introduce an orthonormalized basis by first considering the scalar product of functions (3.6), i.e.,

$$\begin{aligned}&\int \chi_{sLM}^{\lambda *}(\gamma, \vartheta_i)\, \chi_{s'L'M'}^{\lambda'}(\gamma, \vartheta_i)\, d\tau\\ &= \delta_{\lambda\lambda'}\delta_{LL'}\delta_{MM'} 2^{3-\lambda}\pi^{9/2}(2L+1)^{-1}\\ &\quad\times\int_0^\pi \sum_K \phi_K^{\lambda\mu L}(\gamma)\,\phi_K^{\lambda\mu' L}(\gamma)\sin^3\gamma\, d\gamma\\ &= \delta_{\lambda\lambda'}\delta_{LL'}\delta_{MM'} M_{ss'}(\lambda, L),\end{aligned} \tag{5.2}$$

where

$$d\tau = \sin^3\gamma\,\sin\vartheta_2\, d\gamma\, d\vartheta_1\, d\vartheta_2\, d\vartheta_3, \quad 0 \le \vartheta_2,\ \gamma \le \pi, \quad 0 \le \vartheta_1, \vartheta_3 \le 2\pi, \tag{5.3}$$

and the s and μ are related as in (3.9). The matrix $\|M_{ss'}(\lambda, L)\| = \mathbf{M}(\lambda, L)$, for which a program is available[16] is then real and symmetric and thus there exists an orthogonal matrix $\mathcal{O}(\lambda, L) = \|\mathcal{O}_{st}(\lambda, L)\|$ such that

$$\tilde{\mathcal{O}}\,\mathbf{M}\,\mathcal{O} = \mathbf{\Delta} = \|\epsilon_t(\lambda, L)\,\delta_{tt'}\|, \tag{5.4}$$

where ~ indicates transposed and $\mathbf{\Delta}$ is a diagonal matrix whose eigenvalues $\epsilon_t(\lambda, L)$, $t = 1, 2, \ldots, d(\lambda, L)$, are all real and positive. We now define

$$X_{tLM}^\lambda(\gamma, \vartheta_i) = \sum_{s=1}^{d(\lambda,L)} [\epsilon_t(\lambda, L)]^{-1/2}\,\mathcal{O}_{st}(\lambda, L)\,\chi_{sLM}^\lambda(\gamma, \vartheta_i), \tag{5.5}$$

and it is obvious from (5.2), (5.4) that

$$\int X_{tLM}^{\lambda *}(\gamma, \vartheta_i)\, X_{t'L'M'}^{\lambda'}(\gamma, \vartheta_i)\, d\tau = \delta_{\lambda\lambda'}\delta_{tt'}\delta_{LL'}\delta_{MM'}. \tag{5.6}$$

An orthonormal basis that we can use instead of (3.13) may be defined as

$$\begin{aligned}(\alpha_m, \bar{\alpha}\,|\,n\nu\lambda tLM) &= \langle\bar{\alpha}\,|\,n\rangle(\alpha_m\,|\,\nu\lambda tLM)\\ &\equiv \langle\bar{\alpha}\,|\,n\rangle\, F_j^\lambda(\beta)\, X_{tLM}^\lambda(\gamma, \vartheta_i),\end{aligned} \tag{5.7}$$

where $\langle\bar{\alpha}\,|\,n\rangle$ is the one-dimensional harmonic oscillator state of (3.12) while $F_j^\lambda(\beta)$ with $j = (\nu-\lambda)/2$ is given by (3.7). We denote this basis by a round bracket rather than the angular one of (3.13).

It is also convenient to define Wigner coefficients[3] of $O(5) \supset O(3)$ chain of groups in terms of the orthonormalized $X_{tLM}^\lambda(\gamma, \vartheta_i)$ of (5.6) instead of $\chi_{sLM}^\lambda(\gamma, \vartheta_i)$ of (3.6). Thus we write

$$\begin{aligned}&[\lambda tLM, \lambda' t'L'M'\,|\,\lambda'' t''L''M'']\\ &\equiv \int X_{t''L''M''}^{\lambda''*} X_{tLM}^\lambda X_{t'L'M'}^{\lambda'}\, d\tau\\ &= \sum_{ss's''}[\epsilon_{t''}(\lambda'', L'')\,\epsilon_{t'}(\lambda', L')\,\epsilon_t(\lambda, L)]^{-1/2}\\ &\quad\times\mathcal{O}_{s''t''}(\lambda'', L')\,\mathcal{O}_{s't'}(\lambda', L')\,\mathcal{O}_{st}(\lambda, L)\\ &\quad\times\pi^{23/4}\,2^{(6-\lambda-\lambda'-\lambda'')/2}\langle LM, L'M'\,|\,L''M''\rangle\\ &\quad\times(2L''+1)^{-1/2}(-)^{L+L'+L''}(\lambda sL, \lambda' s'L', \lambda'' s''L''),\end{aligned} \tag{5.8}$$

where

$$\begin{aligned}&(\lambda sL, \lambda' s'L', \lambda'' s''L'')\\ &\equiv \int_0^\pi \sum_{KK'K''}\begin{pmatrix} L & L' & L'' \\ K & K' & K''\end{pmatrix}\phi_K^{\lambda\mu L}(\gamma)\,\phi_{K'}^{\lambda'\mu' L'}(\gamma)\\ &\quad\times\phi_{K''}^{\lambda''\mu'' L''}(\gamma)\sin^3\gamma\, d\gamma,\end{aligned} \tag{5.9}$$

and the parenthesis on the right-hand side of (5.9) indicates an ordinary $3j$ symbol of the O(3) group, while the relation between μ and s indices is specified in (3.9).

We now proceed to calculate the matrix elements of Q_M of (5.1) with respect to the states (5.7). To begin with we make use of a simple result due to Hess[17] to write the matrix elements of polynomials in the momentum operators π_m, $\bar{\pi}$ in terms of the corresponding polynomials in the coordinate operators α_m, $\bar{\alpha}$. For this we note that if

$$H_0 \equiv \tfrac{1}{2}\left(\sum_m \pi_m \pi^m + \sum_m \alpha_m \alpha^m\right), \tag{5.10a}$$

$$\bar{H}_0 \equiv \tfrac{1}{2}(\bar{\pi}^2 + \bar{\alpha}^2), \tag{5.10b}$$

then from (2.3)

$$\pi_M = i(H_0 \alpha_M - \alpha_M H_0), \tag{5.11a}$$

$$\bar{\pi} = i(\bar{H}_0 \bar{\alpha} - \bar{\alpha} \bar{H}_0), \tag{5.11b}$$

and thus taking into account that the states (5.7) are eigenstates of H_0, $\bar{H}_0$ with eigenvalues $(\nu + \frac{5}{2})$, $(n + \frac{1}{2})$, respectively, one obtains[17]

$$\begin{aligned}(n''\nu''\lambda''l''L''M''\,|\,\pi_M\bar{\pi}\,|\,n'\nu'\lambda'l'L'M') \\ = -(n'-n'')(\nu'-\nu'')\langle n''|\,\bar{\alpha}\,|n'\rangle \\ \times(\nu''\lambda''l''L''M''|\,\alpha_M\,|\nu'\lambda'l'L'M')\end{aligned} \tag{5.12a}$$

$$\begin{aligned}(n''\nu''\lambda''l''L''M''\,|\,[\pi\times\pi]^2_M\,|n'\nu'\lambda'l'L'M') \\ = (-)^{(\nu''-\nu')/2}\,\delta_{n''n'}(\nu''\lambda''l''L''M''|\,[\alpha\times\alpha]^2_M\,|\nu'\lambda'l'L'M'),\end{aligned} \tag{5.12b}$$

where the last result was obtained by writing $[\pi\times\pi]^2_M$ explicitly and using (5.11a) twice.

When returning to determination of the matrix element of Q_M of (5.1) with respect to the states (5.7) we recall that as this operator is the linear combination (2.13) of generators of U(6), the matrix element must have the selection rule $n'+\nu' = n''+\nu'' = N$. Thus we can finally write

$$\begin{aligned}&(n''\nu''\lambda''l''L''M''\,|\,Q_M\,|n'\nu'\lambda'l'L'M') \\ &= \sqrt{7/3}\,\delta_{\nu'\nu''}\delta_{n''n''}(\nu''\lambda''l''L''M''\,|\,[\alpha\times\alpha]^2_M\,|\nu'\lambda'l'L'M') \\ &\quad + 2\sqrt{4/3}\,\delta_{\nu'+n',\nu''+n''}\langle n''|\,\bar{\alpha}\,|n'\rangle(\nu''\lambda''l''L''M''\,|\,\alpha_M\,|\nu'\lambda'l'L'M').\end{aligned} \tag{5.13}$$

In turn we now write[3]

$$\alpha_M = \beta\chi^1_{12M}(\gamma,\vartheta_i) = c_1\beta X^1_{12M}(\gamma,\vartheta_i), \tag{5.14a}$$

$$[\alpha\times\alpha]^2_M = (1/3\sqrt{7})\,\beta^2\chi^2_{12M}(\gamma,\vartheta_i) = (1/3\sqrt{7})\,c_2\beta^2 X^2_{12M}(\gamma,\vartheta_i), \tag{5.14b}$$

where

$$c_1 = (4\pi/\sqrt{15}), \quad c_2 = 4\pi(6/5)^{1/2}, \tag{5.14c}$$

and in (5.13) we then have to evaluate matrix elements of the form

$$\begin{aligned}&(\nu''\lambda''l''L''M''\,|\,\beta^\lambda X^\lambda_{12M}(\gamma,\vartheta_i)\,|\nu'\lambda'l'L'M') \\ &\quad = \{\lambda''\nu''\,|\,\lambda\,|\,\lambda'\nu'\}[\lambda 12M,\ \lambda'l'L'M'\,|\,\lambda''l''L''M''],\end{aligned} \tag{5.15}$$

where $\lambda = 1, 2$, the curly bracket

$$\{\lambda''\nu''\,|\,\lambda\,|\,\lambda'\nu'\} \equiv \int_0^\infty F^{\lambda''}_{j''}(\beta)\,\beta^\lambda F^{\lambda'}_{j'}(\beta)\,\beta^4\,d\beta \tag{5.16}$$

is given explicitly in Eq. (1.18) of Ref. 2 and the last term is the Wigner coefficient (5.8).

We now wish to obtain explicitly the matrix elements of Q^2 in the basis (5.7), i.e.,

$$\begin{aligned}&(n''\nu''\lambda''l''L''M''\,|\,Q^2\,|n'\nu'\lambda'l'L'M') \\ &= \sum_{n'''\nu'''\lambda'''}\ \sum_M\ \sum_{t'''L'''M'''}(-)^M \\ &\quad\times(n''\nu''\lambda''l''L''M''\,|\,Q_M\,|n'''\nu'''\lambda'''l'''L'''M''') \\ &\quad\times(n'''\nu'''\lambda'''l'''L'''M'''\,|\,Q_{-M}\,|n'\nu'\lambda'l'L'M').\end{aligned} \tag{5.17}$$

These matrix elements clearly contain factors of the form

$$\begin{aligned}&\sum_M\ \sum_{t'''L'''M'''}(-)^M[\lambda 12M,\ \lambda'''l'''L'''M'''\,|\,\lambda''l''L''M''] \\ &\quad\times[\bar{\lambda}12-M,\ \lambda'l'L'M'\,|\,\lambda'''l'''L'''M'''] \\ &= \pi^{23/2}c_\lambda^{-1}c_{\bar{\lambda}}^{-1}\delta_{L'L''}\delta_{M'M''}\sum_{s's''}\ \sum_{s'''\bar{s}'''}\ \sum_{L'''} \\ &\quad\times[\epsilon_{t'}(\lambda',L')\,\epsilon_{t''}(\lambda'',L'')]^{-1/2} \\ &\quad\times O_{s't'}(\lambda',L')O_{s''t''}(\lambda'',L'')\,M^{-1}_{s'''\bar{s}'''}(\lambda''',L''')\,2^{6-\lambda'''} \\ &\quad\times 2^{-(\lambda+\lambda'+\lambda''+\bar{\lambda})/2}[(2L'+1)(2L''+1)]^{-1/2} \\ &\quad\times(\lambda 12,\ \lambda''s''L'',\ \lambda'''s'''L''')(\bar{\lambda}12,\ \lambda's'L',\ \lambda'''s'''L''') \\ &\equiv\langle\lambda''l'''L''\,|\,\lambda\bar{\lambda}\lambda'''\,|\,\lambda'l'L'\rangle\,\delta_{L'L''}\delta_{M'M''},\end{aligned} \tag{5.18}$$

where for the reduction indicated we made use of the orthonormality properties of the ordinary Wigner coefficients appearing in (5.8) and of the fact that from (5.4) we have

$$\begin{aligned}&\sum_{t'''} O_{s'''t'''}(\lambda''',L''')[\epsilon_{t'''}(\lambda''',L''')]^{-1}\tilde{O}_{t'''\bar{s}'''}(\lambda''',L''') \\ &\quad = M^{-1}_{s'''\bar{s}'''}(\lambda''',L'''),\end{aligned} \tag{5.19}$$

where $\mathbf{M}^{-1} \equiv \|M^{-1}_{s'''\bar{s}'''}(\lambda''',L''')\|$ is the reciprocal of the matrix $\mathbf{M}$ whose elements are defined by (5.2). The indices λ, $\bar{\lambda}$ are restricted to the values 1, 2.

We can now write the matrix element of Q^2 as

$$\begin{aligned}&(n''\nu''\lambda''l''LM\,|\,Q^2\,|n'\nu'\lambda'l'LM) \\ &\quad = \tfrac{7}{3}c_2^2\delta_{\nu'\nu''}\delta_{n'n''}\sum_{\lambda'''}\{\lambda''\nu''\,|\,2\,|\,\lambda''\nu''\}\{\lambda'\nu'\,|\,2\,|\,\lambda'''\nu''\} \\ &\quad\times\langle\lambda''l''L\,|\,22\lambda'''\,|\,\lambda'l'L\rangle + (4\sqrt{7}/3)\,c_1c_2\delta_{n'+\nu',n''+\nu''} \\ &\quad\times\sum_{\lambda'''}\{\lambda'''\nu''\,|\,2\,|\,\lambda''\nu''\}\{\lambda'\nu'\,|\,1\,|\,\lambda'''\nu''\}\langle\lambda''l''L\,|\,21\lambda'''\,|\,\lambda'l'L) \\ &\quad\times\langle n''\,|\,\bar{\alpha}\,|n'\rangle + (4\sqrt{7}/3)\,c_1c_2\delta_{n'+\nu',n''+\nu''} \\ &\quad\times\sum_{\lambda'''}\{\lambda'''\nu'\,|\,1\,|\,\lambda''\nu''\}\{\lambda'\nu'\,|\,2\,|\,\lambda'''\nu'\}\langle\lambda''l''L\,|\,12\lambda'''\,|\,\lambda'l'L\rangle \\ &\quad\times\langle n''\,|\,\bar{\alpha}\,|n'\rangle + \tfrac{16}{3}c_1^2\delta_{n'+\nu',n''+\nu''}\sum_{\lambda'''}\Big\{\sum_{\nu'''}[\{\lambda'''\nu'''\,|\,1\,|\,\lambda''\nu''\} \\ &\quad\times\{\lambda'\nu'\,|\,1\,|\,\lambda'''\nu'''\}\langle n''|\,\bar{\alpha}\,|n''+\nu''-\nu'''\rangle\langle n'+\nu'-\nu'''\,|\,\bar{\alpha}\,|n'\rangle] \\ &\quad\times\langle\lambda''l''L\,|\,11\lambda'''\,|\,\lambda'l'L)\Big\},\end{aligned} \tag{5.20}$$

where c_1, c_2 are given by (5.14c), $\{\lambda''\nu''\,|\,\lambda\,|\,\lambda'\nu'\}$ for $\lambda = 1, 2$ is given in (1.18) of Ref. 2 and

$$\langle n''|\,\bar{\alpha}\,|n'\rangle = \left(\frac{n'+1}{2}\right)^{1/2}\delta_{n'',n'+1} + \left(\frac{n'}{2}\right)^{1/2}\delta_{n'',n'-1}. \tag{5.21}$$

The factor $\langle \lambda'' l'' L | \lambda \bar{\lambda} \lambda''' | \lambda' l' L' \rangle$ is defined by (5.18) in terms of the reduced $3j$ symbols (5.9), already programmed[16] for $\lambda = 1, 2$, and the matrices $O(\lambda, L) = \| O_{st}(\lambda, L) \|$, $\Delta(\lambda, L) = \| \epsilon_t(\lambda, L)\, \delta_{tt'} \|$ required in the orthonormal basis.

We have thus obtained explicitly the matrix elements of Q^2 in the basis (5.7) and in the next section we indicate some of their applications and the available programs for determining them numerically.

Finally we wish to discuss how far a definite eigenvalue of Q^2 fixes the irreducible representation of the group SU(3). For this purpose we recall that a representation of U(3) can be characterized by a partition $[h_1 h_2 h_3]$, $h_1 \geq h_2 \geq h_3 \geq 0$. The number operator in U(3) is given by[10]

$$\sum_{l'm'} \sum_{l''m''} \langle 2l'm' | H_0 - \tfrac{3}{2} | 2l''m'' \rangle\, \eta_{l'm'} \xi^{l''m''} = 2\hat{N}, \tag{5.22}$$

where H_0 is the Hamiltonian of a three-dimensional oscillator, and thus the matrix elements are $2\delta_{l'l''}\delta_{m'm''}$. Thus the partition characterizing the irreducible representation of U(3) is restricted by the relation

$$h_1 + h_2 + h_3 = 2N. \tag{5.22a}$$

Furthermore the second order Casimir operator G of U(3) given in (2.21) has eigenvalues g of the form[10]

$$g = h_1^2 + h_2^2 + h_3^2 + 2h_1 - 2h_3. \tag{5.23}$$

Thus if we designate by q^2 an eigenvalue of Q^2 we obtain from (2.21) and (5.23) that

$$q^2 = h_1^2 + h_2^2 + h_3^2 + 2h_1 - 2h_3 - \tfrac{1}{2}L(L+1) - \tfrac{4}{3}N^2. \tag{5.22b}$$

Clearly then if N, q^2, L are specified we have two equations for the three unknowns h_1, h_2, h_3. We note though that h_1, h_2, h_3 are integers satisfying the inequalitites $h_1 \geq h_2 \geq h_3 \geq 0$ and thus the possibility of several solutions of the equations (5.22) is severely limited. This limitation is enhanced when we take into account that $[h_1 h_2 h_3]$ is a representation of U(3) contained in the representation N of U(6). Discussions by several authors[8,11,18] then indicate that $[h_1 h_2 h_3]$ take the form

$$h_3 = 2y, \quad h_2 = 2(x+y), \quad h_1 = 2(N - x - 2y), \tag{5.24}$$

where x and y are integers satisfying the inequalities

$$0 \leq x \leq [N/2], \quad 0 \leq y \leq [(N - 2x)/3], \tag{5.25}$$

with $[\ ]$ meaning the integer closest from below to the number inside the bracket.

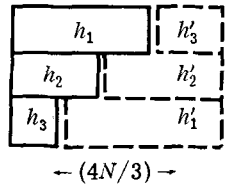
Even with the above limitations Eq. (5.22b) may be solved by more than one pair of x, y. To see this we first rewrite the Eq. (5.22b) using (5.22a) as

$$q^2 = \tfrac{2}{3}(p^2 + rp + r^2) + 2(r+p) - \tfrac{1}{2}L(L+1), \tag{5.26}$$

where

$$p \equiv h_1 - h_2 = 2(N - 2x - 3y), \quad r \equiv h_2 - h_3 = 2x, \tag{5.27}$$

and thus (p, r) characterizes an irreducible representation in the fashion of Elliott[11] who uses the notation (λ, μ), which we avoid, as these letters have another meaning in the present paper. Clearly (5.26) remains invariant if we interchange p and r, and thus for N divisible by 3 we can consider the conjugate partitions



(5.28)

for which

$$p = h_1 - h_2 = h_2' - h_3' = r', \quad r = h_2 - h_3 = h_1' - h_2' = p', \tag{5.29}$$

and so they correspond to the same q^2.

For N divisible by 3 the two irreducible representations of U(3) given by

$$[2N - 2x - 4y, 2x + 2y, 2y], \tag{5.30a}$$

$$[\tfrac{4}{3}N - 2y, \tfrac{4}{3}N - 2x - 2y, 2x + 4y - \tfrac{2}{3}N], \tag{5.30b}$$

are contained in the irreducible representation N of U(6) if $(2x + 4y - \frac{2}{3}N) \geq 0$ and the partitions are not identical; in that case they correspond to the same q^2. Thus the states obtained by diagonalization of Q^2 will be linear combinations of them as, for example, happens when $N = 6$, where $[h_1 h_2 h_3]$ takes the values

$$[12, 00] \oplus [10, 20] \oplus [840] \oplus [\underline{822}] \oplus [\underline{660}] \oplus [642] \oplus [444], \tag{5.31}$$

and the partitions underlined have the same q^2 as they meet the conditions mentioned above.

So far we have not been able to detect other types of degeneracy in the U(3) representation, but in any case their presence will not be relevant for the kind of applications discussed in the concluding section.

6. THE INTERACTING BOSON MODEL

The most general two-body interaction involving d and s bosons can be expressed in the form[10]

$$\begin{aligned} V &= \tfrac{1}{2} \sum_{l_1 m_1 l_2 m_2} \sum_{l_1' m_1' l_2' m_2'} \{ \langle 2l_1 m_1, 2l_2 m_2 | V_{12} | 2l_1' m_1', 2l_2' m_2' \rangle \\ &\quad \times \eta_{l_1 m_1} \eta_{l_2 m_2} \xi^{l_1' m_1'} \xi^{l_2' m_2'} \} \\ &= \tfrac{1}{2} \sum_{l_1 l_2} \sum_{l_1' l_2'} \sum_{L} \{ \langle 2l_1, 2l_2, L | V_{12} | 2l_1', 2l_2', L \rangle \\ &\quad \cdot (-)^{l_1' + l_2'} (2L+1)^{1/2} [[\eta_{l_1} \times \eta_{l_2}]^L \times [\xi_{l_1'} \times \xi_{l_2'}]^L]_0^0 \}, \end{aligned} \tag{6.1}$$

where $|2lm\rangle$ is an harmonic oscillator state of two quanta so that l is restricted to the values $l = 0, 2$, and in the last part of (6.1) we recoupled bra and ket to a total L, assuming of course that V_{12} is invariant under rotations.

If the matrix elements in (6.1) are real, as happens for example[19] if $V_{12} = V(|\mathbf{r}_1 - \mathbf{r}_2|)$, then a brief examination of it indicates that we have only seven types of independent Hermitian interactions that we proceed to write down in the notation (2.6)

$$A_L \equiv [[\eta \times \eta]^L \times [\xi \times \xi]^L]_0^0, \quad L = 0, 2, 4, \tag{6.2a}$$

$$B \equiv [\eta \times \xi]^0_0 \bar{\eta}\bar{\xi}, \tag{6.2b}$$

$$C \equiv \bar{\eta}^2 \bar{\xi}^2, \tag{6.2c}$$

$$D \equiv [\eta \times \eta]^0_0 \bar{\xi}^2 + \bar{\eta}^2 [\xi \times \xi]^0_0, \tag{6.2d}$$

$$E \equiv [[\eta \times \eta]^2 \times \xi]^0_0 \bar{\xi} + \bar{\eta}[\eta \times [\xi \times \xi]^2]^0_0. \tag{6.2e}$$

The A_L, $L = 0, 2, 4$, are the independent interactions involving only d bosons, and already in the initial work of Arima and Iachello[6] it was shown that they can be expressed in terms of $\hat{N}^2$, $\hat{N}$, Λ^2 and L^2. The B, C can obviously be expressed in terms of $\hat{N}$, $\hat{\mathcal{N}}$ of (2.15) while D is related with the K^2 of (2.18) and thus with $\mathcal{L}^2 - \Lambda^2$. There remains then to determine E for which we first consider the operator $Q^2 = \sum_m (-)^m Q_m Q_{-m}$ taking for Q_m the expression (2.13), i.e.,

$$\begin{aligned} Q^2 &= \sqrt{5}[\mathbf{Q} \times \mathbf{Q}]^0_0, \\ &= \sqrt{5}\{\tfrac{7}{3}[[\eta \times \xi]^2 \times [\eta \times \xi]^2]^0_0 \\ &\quad + \tfrac{4}{3}\sqrt{7}[[\eta \times \xi]^2 \times (\eta \bar{\xi} + \bar{\eta}\xi)]^0_0 \\ &\quad + \tfrac{4}{3}[(\eta \bar{\xi} + \bar{\eta}\xi) \times (\eta \bar{\xi} + \bar{\eta}\xi)]^0_0\}. \end{aligned} \tag{6.3}$$

Straightforward recoupling then shows that Q^2 takes the form

$$\begin{aligned} Q^2 = \tfrac{35}{3} \sum_L W(2222; 2L)\sqrt{2L+1}\, A_L + \tfrac{7}{3}\hat{\mathcal{N}} \\ + \tfrac{4}{3}\sqrt{35}\, E + \tfrac{4}{3}[2\hat{\mathcal{N}}(\hat{N} - \hat{\mathcal{N}} + 1) + 2(\hat{\mathcal{N}} + 5)(\hat{N} - \hat{\mathcal{N}}) - K^2], \end{aligned} \tag{6.4}$$

where $\hat{\mathcal{N}}$, $\hat{N}$, and K^2 are given respectively by (2.15) and (2.18) and W is a Racah coefficient. Obviously then we can express E in terms of Q^2 and the other Casimir operators of the groups in the chains (1.1), (1.2). In the following equations we given explicitly the form of all the interactions (6.2) in terms of the Casimir operators mentioned:

$$A_0 = \tfrac{1}{5}\hat{\mathcal{N}}(\hat{\mathcal{N}} + 3) - \tfrac{1}{5}\Lambda^2, \tag{6.5a}$$

$$A_2 = \frac{1}{7\sqrt{5}}\{-\mathbf{L}^2 + 2\Lambda^2 + 2\hat{\mathcal{N}}(\hat{\mathcal{N}} - 2)\}, \tag{6.5b}$$

$$A_4 = \tfrac{1}{7}\{\tfrac{1}{3}\mathbf{L}^2 - \tfrac{1}{5}\Lambda^2 + \tfrac{6}{5}\hat{\mathcal{N}}(\hat{\mathcal{N}} - 2)\}, \tag{6.5c}$$

$$B = \frac{1}{\sqrt{5}}(\hat{N} - \hat{\mathcal{N}})\hat{\mathcal{N}}, \tag{6.5d}$$

$$C = (\hat{N} - \hat{\mathcal{N}})(\hat{N} - \hat{\mathcal{N}} - 1), \tag{6.5e}$$

$$D = \frac{1}{\sqrt{5}}\{\Lambda^2 - \mathcal{L}^2 + 2\hat{N}\hat{\mathcal{N}} - 2\hat{\mathcal{N}}^2 + 5\hat{N} - 4\hat{\mathcal{N}}\}, \tag{6.5f}$$

$$\begin{aligned} E = \frac{3}{4\sqrt{35}}\{Q^2 - \tfrac{2}{3}\Lambda^2 + \tfrac{4}{3}\mathcal{L}^2 - \tfrac{1}{6}\mathbf{L}^2 + \tfrac{14}{3}\hat{\mathcal{N}}^2 \\ + \tfrac{22}{3}\hat{\mathcal{N}} - \tfrac{8}{3}\hat{N}(2\hat{\mathcal{N}} + 5)\}. \end{aligned} \tag{6.5g}$$

From the discussion in the previous sections it is clear that we can write the matrix elements of an arbitrary interaction in the basis of states (5.7) characterized by the irreducible representations of the chain of groups $U(6) \supset U(5) \supset O(5) \supset O(3)$. From a numerical standpoint the only stumbling block is the matrix element (5.20) of Q^2 for which already the reduced $3j$ symbols $(112; \lambda' s' L'; \lambda'' s'' L'')$, $(212; \lambda' s' L'; \lambda'' s'' L'')$ have been programmed as well as $M_{ss'}(\lambda, L)$ which is proportional to $(000; \lambda s L; \lambda s' L)$. What remains to be done is to assemble a full numerical program for the matrix elements of Q^2, which hopefully will be achieved soon.[16]

Thus we claim that the group theory, as well as a good part of the numerical analysis, for general problems in the interacting boson model, is now available.

Note added in proof: Since submission of this paper we have found an alternative procedure for the determination of the matrix elements (m.e.) of the operator Q^2, which is simpler than the method discussed in Sec. 5. From (6.5g) we can see that the operator Q^2 is a linear combination of $\mathcal{L}^2$, E, plus operators diagonal in the basis (3.13). As the m.e. of $\mathcal{L}^2$ in that basis were given in (4.9), (4.10), if we construct the matrix of the operator E of (6.2e) with respect to the states (3.13) we shall have available the matrix of Q^2. The operator E is the sum of two terms, each one being the Hermitian conjugate of the other, hence it is sufficient to find the m.e. of the first term, i.e., $[[\eta \times \eta]^2 \times \xi]^0_0 \bar{\xi}$, from which the m.e. of the second term follow easily. The action of the boson operator $\bar{\xi}$ on the state (3.13) was given in Eq. (4.6); thus it remains only to determine the action of $[[\eta \times \eta]^2 \times \xi]^0_0$ on the $U(5) \supset O(5)$ states of (3.5).

For this last task we use the definitions (2.4) and properties of Clebsch–Gordan coefficients of O(3) to show that

$$\begin{aligned} 2\sqrt{2}\,[[\alpha \times \alpha]^2 \times \alpha]^0_0 = \\ [[\eta \times \eta]^2 \times \eta]^0_0 + 3[[\eta \times \eta]^2 \times \xi]^0_0 \\ + 3[[\xi \times \xi]^2 \times \xi]^0_0. \end{aligned} \tag{i}$$

Taking the m.e. of this identity with respect to states (3.5) with ν and $\nu + 1$ quanta of energy, we deduce

$$\begin{aligned} \langle \nu + 1, \lambda' s' L M | [[\eta \times \eta]^2 \times \xi]^0_0 | \nu \lambda s L M \rangle \\ = -\frac{4}{3\sqrt{35}} \langle \nu + 1, \lambda' s' L M | \beta^3 \cos 3\gamma | \nu \lambda s L M \rangle, \end{aligned} \tag{ii}$$

where we have used[2,3]

$$[[\alpha \times \alpha]^2 \times \alpha]^0_0 = \frac{1}{\sqrt{35}}\{3, 0\} = -\sqrt{2/35}\,\beta^3 \cos 3\gamma. \tag{iii}$$

The m.e. (ii) factorizes into a product of the m.e. of β^3 with respect to the functions (3.7), for which a closed formula is known,[2] times the m.e. of $\cos 3\gamma$ with respect to the functions (3.6), this being proportional to the reduced $3j$ symbol $(310, \lambda' s' L, \lambda s L)$ defined in (5.9) and for which computer programs are already available.

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APPENDIX A: NORMALIZATION COEFFICIENTS IN THE CHAIN U(6) ⊃ O(6)

In this Appendix we shall determine the value of the

normalization coefficient $B_{N\rho\lambda}$ appearing in Eq. (4.16). We choose this coefficient in such a way that the functions in Eq. (4.16) possess orthonormality properties with respect to the indices N, ρ whenever $g_\lambda^\rho(\delta)$ and $f^\rho_{(N-\rho)/2}(b)$ are defined according to Eqs. (4.19) and (4.20).

From Ref. 15, pp. 827, 844 we have:

$$\int_0^\pi (\sin\delta)^{2\lambda+4} C_{\rho-\lambda}^{\lambda+2}(\cos\delta)\, C_{\rho'-\lambda}^{\lambda+2}(\cos\delta)\, d\delta = \frac{\pi(\rho+\lambda+3)!\,\delta_{\rho\rho'}}{(\rho+2)\,2^{2\lambda+3}(\rho-\lambda)!\,(\lambda+1)^2}, \tag{A1}$$

$$\int_0^\infty \exp(-b^2)\, b^{2\rho+5} L^{\rho+2}_{(N-\rho)/2}(b^2)\, L^{\rho+2}_{(N'-\rho)/2}(b^2)\, db = [(N+\rho)/2+2]!\,/2[(N-\rho)/2]!\;\delta_{NN'}. \tag{A2}$$

From here, as well as from the definition of $g(\delta)$ and $f(b)$ in (4.19), (4.20), it immediately follows that if we take

$$B_{N\rho\lambda} = 2^{\lambda+2}(\lambda+1)! \left[\frac{(\rho-\lambda)!\,[(N-\rho)/2]!\,(\rho+2)}{\pi(\rho+\lambda+3)!\,[(N+\rho)/2+2]!}\right]^{1/2}, \tag{A3}$$

then the $U(6)\supset O(6)\supset O(5)$ kets $|N\rho\lambda sLM\rangle$ of Eq. (4.16) will be orthonormal in the indices N, ρ. The corresponding "volume element" in b, δ is $b^5(\sin\delta)^4\, db\, d\delta$.

APPENDIX B: TRANSFORMATION BRACKETS BETWEEN STATES IN THE CHAIN U(6) ⊃ O(6) ⊃ O(5) AND U(6) ⊃ U(5) ⊃ O(5)

The states characterized by irreducible representations of the chain of groups $U(6)\supset U(5)\supset O(5)\supset O(3)$ are given by (3.13) and (3.5), while those in the chain $U(6)\supset O(6)\supset O(5)\supset O(3)$ take the form (4.16). As we want to develop the latter in terms of the former it is clear that the transformation bracket is independent of s, L, M and diagonal in λ[20]; thus for a given λ we can choose

$$s=1, \quad L=M=2\lambda. \tag{B1}$$

The states corresponding to the two chains specified above can then be characterized by the kets $|n\nu\lambda\rangle$ and $|N\rho\lambda\rangle$ given respectively by

$$|n\nu\lambda\rangle = \langle\overline{\alpha}\,|n\rangle \left[2\left(\frac{\nu-\lambda}{2}\right)!\Big/\Gamma\left(\frac{\nu+\lambda+5}{2}\right)\right]^{1/2} \times L^{\lambda+3/2}_{(\nu-\lambda)/2}(\beta^2)\exp(-\beta^2/2)\,\alpha_2^\lambda, \tag{B2a}$$

$$|N\rho\lambda\rangle = B_{N\rho\lambda}\, b^\rho\, L^{\rho+2}_{(N-\rho)/2}(b^2)\exp(-b^2/2) \times (\sin\delta)^\lambda\, C_{\rho-\lambda}^{\lambda+2}(\cos\delta)(\alpha_2/\beta)^\lambda, \tag{B2b}$$

where $\langle\overline{\alpha}\,|n\rangle$ is the one-dimensional harmonic oscillator state (3.12), and we made use of the fact that[3]

$$\chi^\lambda_{1,2\lambda,2\lambda}(\gamma,\vartheta_i) = \left(\frac{\alpha_2}{\beta}\right)^\lambda. \tag{B3}$$

As the function χ is not normalized with the volume element (5.3), we would need to multiply the kets (B2) by the $M_{11}^{-1/2}(\lambda, 2\lambda)$ defined in (5.2) if the kets themselves are normalized. As this factor would appear both in (B2a) and (B2b) we do not include it.

Instead of trying to do the expansion of $|N\rho\lambda\rangle$ in terms of $|n\nu\lambda\rangle$ using the expressions given in (B2), it is rather simpler to make the whole analysis using alternative realizations for those states in terms of the boson operators η_m, $\overline{\eta}$ of Eq. (2.4). We proceed now to obtain these expressions. In their derivation use will be made of two facts:

(i) If

$$P_\lambda(\alpha_1,\ldots,\alpha_r)\exp[-(\boldsymbol{\alpha}\cdot\boldsymbol{\alpha})/2], \quad (\boldsymbol{\alpha}\cdot\boldsymbol{\alpha}) = \sum_{i=1}^r \alpha_i^2 \tag{B4}$$

is a normalized r-dimensional harmonic-oscillator wavefunction of λ quanta of energy which is an eigenfunction of the Casimir operator of $O(r)$ with eigenvalue $\lambda(\lambda+r-2)$, then

$$\pi^{r/4}2^{-\lambda/2}P_\lambda(\eta_1,\ldots,\eta_r)\,|0\rangle \tag{B5}$$

is a normalized state with the same quantum numbers as (B4); this is Dragt's theorem.[2,21]

(ii) For the polynomial appearing in (B5) and for any positive integer p we have, with a notation for scalar product similar to that in (B4),

$$(\xi\cdot\xi)(\eta\cdot\eta)^p P_\lambda(\eta)\,|0\rangle = 2p(2p+r-2+2\lambda)(\eta\cdot\eta)^{p-1}P_\lambda(\eta)\,|0\rangle. \tag{B6}$$

This relation is a consequence of $(\xi\cdot\xi)P_\lambda(\eta)\,|0\rangle = 0$, and the equivalence $\xi_i P(\eta)\,|0\rangle = (\partial/\partial\eta_i)P(\eta)\,|0\rangle$.

For the case of the $U(6)\supset U(5)$ states of (B2a), we deduce from Dragt's theorem,

$$|0\lambda\lambda\rangle = \left[\frac{2}{\Gamma(\lambda+5/2)}\right]^{1/2}\pi^{5/4}2^{-\lambda/2}\,\eta_2^\lambda\,|0\rangle, \tag{B7}$$

where we want to remark that we have omitted on the right-hand side of (B7) the same factor $M_{11}^{-1/2}(\lambda,2\lambda)$ that was ignored in Eqs. (B2). Then, from (5.4) of Ref. 1,

$$|0\nu\lambda\rangle = B'_{\nu\lambda}\left[\frac{2}{\Gamma(\lambda+5/2)}\right]^{1/2}\pi^{5/4}2^{-\lambda/2}(\eta\cdot\eta)^{(\nu-\lambda)/2}\eta_2^\lambda\,|0\rangle \tag{B8}$$

where the coefficient $B'_{\nu\lambda}$ is evaluated by repeated application of Eq. (B6), leading to the result

$$B'_{\nu\lambda} = (-)^{(\nu-\lambda)/2}\left[\frac{[(\nu+\lambda)/2+1]!\,(2\lambda+3)!}{[(\nu-\lambda)/2]!(\lambda+1)!\,(\nu+\lambda+3)!}\right]^{1/2}, \tag{B9}$$

Finally, it is quite obvious that

$$|n\nu\lambda\rangle = (n!)^{-1/2}(\overline{\eta})^n\,|0\nu\lambda\rangle. \tag{B10}$$

The phase factor that we have attached to $B'_{\nu\lambda}$ in Eq. (B9) was chosen in such a way that (B10) has exactly the same phases as (B2a). The proof of this assertion can be given by a reasoning similar to that presented in Sec. 9 of Ref. 13; we shall omit it here.

Turning now to the $U(6)\supset O(6)$ states of (B2b), from Dragt's theorem we obtain

$$|\rho\rho\lambda\rangle = B_{\rho\rho\lambda}\pi^{3/2}2^{\rho/2-\lambda}\,\frac{(\rho+1)!}{(\rho-\lambda)!\,(\lambda+1)!}\,\eta_2^\lambda\sum_s a_s(\overline{\eta})^{\rho-\lambda-2s} \times(\eta\cdot\eta+\overline{\eta}^2)^s\,|0\rangle, \tag{B11}$$

where $B_{\rho\rho\lambda}$ is given in Eq. (A3), and

$$a_s = \left(\frac{\lambda-\rho}{2}\right)_s \left(\frac{\lambda-\rho+1}{2}\right)_s \Big/ s!\,(-\rho-1)_s, \tag{B12}$$

are coefficients coming from the power series expansion of the Gegenbauer polynomial $C_{\rho,\lambda}^{\lambda+2}(\cos\delta)$ (formula 8.932.1b of Ref. 15), $(\chi)_s \equiv \chi(\chi+1)\cdots(\chi+s-1)$ is the Pochhammer symbol. Again, we are omitting a factor $M_{11}^{-1/2}(\lambda, 2\lambda)$ on the right-hand side of (B11). By analogy with (B8), the general state is now

$$|N\rho\lambda\rangle = B'_{N\rho}(\boldsymbol{\eta}\cdot\boldsymbol{\eta}+\overline{\eta}^2)^{(N-\rho)/2}|\rho\rho\lambda\rangle, \tag{B13}$$

where $B'_{N\rho}$ is determined by repeated use of Eq. (B.6) which gives

$$B'_{N\rho} = (-)^{(N-\rho)/2}\left[\frac{(\rho+2)!}{2^{N-\rho}((N-\rho)/2)!\,((N+\rho)/2+2)!}\right]^{1/2}. \tag{B14}$$

The phase factor in (B14) was again determined in such a way that (B13) and (B2b) have exactly the same phases.

The last step in our analysis consists in the expansion of the binomial $(\boldsymbol{\eta}\cdot\boldsymbol{\eta}+\overline{\eta}^2)^{s+(N-\rho)/2}$ that appears in (B13) when one introduces there the explicit expression (B11) for $|\rho\rho\lambda\rangle$. After an interchange of sums, by comparison with (B10) it is deduced that

$$|N\rho\lambda\rangle = \sum_{\nu}\langle n\nu\lambda|N\rho\lambda\rangle\,|n\nu\lambda\rangle, \quad \nu-\lambda \text{ even}, \tag{B15}$$

with $\langle n\nu\lambda|N\rho\lambda\rangle$ given by Eq. (4.21).

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Exact solutions of some multiplicative stochastic processes

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The theory of multiplicative stochastic processes with completely and quasicompletely random Gaussian statistics is discussed. Operator valued equations with stochastic coefficients are solved exactly for various types of statistics using the path integral technique. Generalizations of previous results for such stochastic processes are obtained.

I. INTRODUCTION

The first applications of random processes in physics were mostly concerned with the so called additive stochastic processes. From a mathematical point of view such stochastic processes are described by linear integrodifferential equations with the inhomogeneity as the random variable of the process.

A harmonic oscillator with a random driving force $F(t)$:

$$\frac{db}{dt} = -i\omega_0 b + iF(t) \tag{1.1}$$

is a simple example of an additive stochastic process. Such processes were studied extensively in the past in the theory of Brownian motion or in the theory of random-noise currents in electronical devices.[1]

In many physical situations we have to deal with equations with a much more complicated dependence on the random variables. For example, the harmonic oscillator from Eq. (1.1) can be driven by the random force $F(t)$ in the following way:

$$\frac{db}{dt} = -i\omega_0 b + iF(t)b^*, \tag{1.2}$$

i.e., the random variable instead of being the inhomogeneity, multiplies the oscillator operator b^*. Equation (1.2) is only an example of a wider class of stochastic processes for which the random variable enter in a multiplicative way. Such processes are called multiplicative stochastic processes (MSP) and have been studied in Ref. 2.

Many physical applications of MSP can be found for example in the theory of magnetic resonance.[3,4] In the last two years or so the multiplicative stochastic processes have been applied in atomic physics in order to describe different incoherence effects of atoms coupled to a laser field. One of the first application of this theory to atomic problems was done in the framework of a two-level atom coupled to a stochastic electromagnetic field with a stochastic random phase.[5] In a different context, it has been shown that the QED atomic Heisenberg equations of motion describing an atom coupled to a quantized electromagnetic field have the formal form of a multiplicative stochastic process with the free-field operator of the electromagnetic field as the "random" variable.[6]

It turns out that the entire class of problems of interest in the theory of MSP can be written in the form of the following operator-valued equation

$$\frac{d\psi}{dt} = M_0\psi + ix(t)M_1\psi + ix^*(t)M_2\psi, \tag{1.3}$$

where ψ is an operator-valued vector of dimension n with $x(t)$ and $x^*(t)$ being two complex stochastic processes. The matrices M_0, M_1, and M_2 are in general complex, time independent and of the order $n\times n$. In this paper we solve Eq. (1.3) exactly for stochastic processes of Gaussian type. In our approach we use the path-integral technique in order to find explicit solutions and to avoid tedious calculations performed in previous references.

In Sec. II we introduce our notation and define the class of stochastic processes by a proper definition of the functional measure in the proper path integral. Next we define a class of the so-called quasicompletely random processes for which exact solution of Eq. (1.3) can be obtained. These processes have not been discussed previously.

In Sec. III we obtain exact solutions of our problem applying path-integral techniques together with scattering-theory methods. Exact solutions are produced even for cases when Eq. (1.13) has a stochastic dependent initial boundary condition. In Sec IV a simple example of the theory is solved as an illustration of the method. Finally, some concluding remarks are presented. The results of this paper are the generalization of the theory of MSP presented in Ref. 2. The initial boundary condition stochastic dependence and the quasi-completely random processes have not been discussed so far in the literature. All these problem started to be important in the theory of incoherence effects in atomic photophysics.

II. GENERATING FUNCTIONS AND PATH INTEGRATION

To define a random process we have to introduce the statistical properties of the random variables $x(t)$ and $x^*(t)$. This can be done in a twofold way. We can assume an infinite set of all possible correlation functions of x and x^* or we can define in the space of all possible realizations of x and x^* a probability measure with respect to which the stochastic average should be calculated. For any arbitrary dynamical variable $\mathcal{J}[x,x^*]$ which is a functional of the stochastic variables x and x^* we define the following stochastic average:

$$\langle \mathcal{J} \rangle = \int \mathcal{D}\mu[x,x^*]\mathcal{J}[x,x^*]. \tag{2.1}$$

In this equation a functional integration[7] (path-integral) over all possible relaizations of the random variables x and x^* is performed. In order to have a Gaussian

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process we assume that the functional measure $D\mu[x,x^*]$ has a Gaussian density

$$D\mu[x,x^*]=N^{-1}DxDx^* \times\exp\left[-\tfrac{1}{2}\int d\tau_1 d\tau_2 (x(\tau_1),x^*(\tau_2))K(\tau_1,\tau_2)\begin{pmatrix}x(\tau_1)\\ x^*(\tau_2)\end{pmatrix}\right], \quad (2.2)$$

where $K(\tau_1,\tau_2)$ is an arbitrary positive 2×2 integral kernel and N is a normalization factor to assure $\int D\mu[x,x^*]=1$. For quadratic density measure the functional integration can be done exactly. For example, the characteristic function

$$Z[\mathcal{J},\mathcal{J}^*]=\langle\exp[i\int d\tau x(\tau)\mathcal{J}^*(\tau)+i\int d\tau x^*(\tau)\mathcal{J}(\tau)]\rangle, \quad (2.3)$$

with J and J^* arbitrary functions has the following form[8]:

$$Z[\mathcal{J},\mathcal{J}^*] =\exp\left[-\tfrac{1}{2}\int d\tau_1 d\tau_2 (\mathcal{J}^*,\mathcal{J}(\tau_2))(\tau_1\tau_2)\begin{pmatrix}\mathcal{J}^*(\tau_2)\\ \mathcal{J}(\tau_2)\end{pmatrix}\right] \quad (2.4)$$

where the integral kernel $\Delta(\tau_1,\tau_2)$ is a 2×2 matrix, inverse to the matrix $K(\tau_1,\tau_2)$:

$$\int d\tau_1 \Delta(\tau_1,\tau_3)K(\tau_3,\tau_2)=\delta(\tau_1-\tau_2). \quad (2.5)$$

The measure (2.2) defines the random process completely. By a proper choice of the functions K we can generate different Gaussian statistics of the random variables x and x^*. All the correlation functions of the random process can be than computed from Eq. (2.3) by functional differentiation of the characteristic function $Z[\mathcal{J},\mathcal{J}^*]$ given by Eq. (2.4). For example, we have

$$\langle x(t)\rangle=(-i)\frac{\delta Z}{\delta\mathcal{J}^*(t)}\bigg|_{\mathcal{J}=\mathcal{J}^*=0}=0,$$

$$\langle x^*(t)\rangle=(-i)\frac{\delta Z}{\delta\mathcal{J}(t)}\bigg|_{\mathcal{J}=\mathcal{J}^*=0}=0, \quad (2.6a)$$

$$\langle x(t)x(s)\rangle=(-i)^2\frac{\delta^2 Z}{\delta\mathcal{J}^*(t)\delta\mathcal{J}^*(s)}\bigg|_{\mathcal{J}=\mathcal{J}^*=0} =\tfrac{1}{2}(\Delta_{22}(t_1s)+\Delta_{22}(s_1t)), \quad (2.6b)$$

$$\langle x(t)x^*(s)\rangle=(-i)^2\frac{\delta^2 Z}{\delta\mathcal{J}^*(t)\delta\mathcal{J}(s)}\bigg|_{\mathcal{J}=\mathcal{J}^*=0} =\tfrac{1}{2}(\Delta_{12}(t_1s)+\Delta_{21}(s_1t)). \quad (2.6c)$$

In Eqs. (2.6) the expressions $\Delta_{ij}(t,s)$ with $i,j=1,2$ are the proper matrix elements of the matrix $\Delta(t,s)$. A completely random process corresponds to the following choice of the Δ's functions:

$$\Delta_{ij}(t,s)=2D_{ij}\delta(t-s), \quad i,j=1,2, \quad (2.7)$$

where D_{ij} are constant coefficients. For the purpose of this paper and further physical applications we are going to generalize Eq. (2.7) using the following formal finite series expansion of the Δ functions:

$$\Delta_{ij}(t,s)=\sum_{n=0}^{N}\Gamma_{ij}^n\frac{d^{2n}}{dt^{2n}}\delta(t-s). \quad (2.8)$$

The class of stochastic processes with correlation functions given by Eq. (2.8) is called quasicompletely random processes. The expansion (2.8) truncated to the first term with $n=0$ describes a completely random process given by Eq. (2.7). The expansion given by Eq. (2.8) can be obtained, for example, from the following physical arguments.

Let Δ_{ij} be stationary correlation functions with symmetric power spectrum:

$$\Delta_{ij}(t,s)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-s)}\tilde{\Delta}_{ij}(\omega), \quad \tilde{\Delta}_{ij}(\omega)=\tilde{\Delta}_{ij}(-\omega). \quad (2.9)$$

In many physical applications, the power spectrum of the stochastic process is a Lorentzian function centered around $\omega=0$, and with a bandwidth Γ_{ij}:

$$\tilde{\Delta}_{ij}(\omega)=\frac{2\Gamma_{ij}}{\omega^2+\Gamma_{ij}^2} \quad (2.10)$$

Now the relation (2.8) can be obtained by a formal Taylor expansion of the power-spectrum functions

$$\tilde{\Delta}_{ij}(\omega)=\tilde{\Delta}_{ij}(0)+\frac{\omega^2}{2!}\frac{d^2\tilde{\Delta}_{ij}}{d\omega^2}\bigg|_{\omega=0}+\frac{\omega^4}{4!}\frac{d^4\tilde{\Delta}_{ij}}{d\omega^4}\bigg|_{\omega=0}+\cdots. \quad (2.11)$$

The Fourier integration of the expansion (2.11) leads to a quasicompletely random process with the following coefficients Γ_{ij}^n:

$$\Gamma_{ij}^n=\frac{(-1)^n}{(2n)!}\frac{d^{2n}\tilde{\Delta}_{ij}}{d\omega^{2n}}\bigg|_{\omega=0}. \quad (2.12)$$

We have truncated the sum in Eq. (2.8) to a finite number N of terms to avoid problems with convergence. The series expansion (2.8) should be understood as an asymptotic approximation of the functions.

If the Lorentzian given by Eq. (2.10) has a very sharp power spectrum, i.e., $\Gamma_{ij}\to 0$, we can keep in the expansion (2.8) only the first term with $\Gamma_{ij}^0=2D_{ij}$. In this limit the process becomes completely random [see Eq. (2.7)]. Higher corrections coming from the fact that Γ_{ij} is finite may be calculated in a systematic way using the expansion (2.8).

In general, however, we can adopt Eq. (2.8) as the definition of quasicompletely random processes without any particular justification based on the power-spectrum properties.

III. SOLUTIONS OF STOCHASTIC EQUATIONS

Our goal in this section is an exact expression for the following stochastic average:

$$\langle\psi\rangle=\int D\mu[x,x^*]\psi[x,x^*], \quad (3.1)$$

with $\psi[x,x^*]$ satisfying the evolution equation (1.3). We can get rid the statistically independent part of the evolution in this equation, introducing the "interaction picture" transformation:

$$\psi_I(t)=e^{-M_0t}\psi(t). \quad (3.2)$$

This transformation leads to the following equation:

$$\frac{d\psi_I}{dt}=[ix(t)M_1(t)+ix^*(t)M_2(t)]\psi_I, \quad (3.3)$$

with

$$M_1(t)=e^{-M_0t}M_1e^{M_0t}, \quad M_2(t)=e^{-M_0t}M_2e^{M_0t}. \quad (3.4)$$

We can now write the solution of Eq. (3.3) in the following form:

$$\psi_I(t)=T\exp[i\int_0^t d\tau(x(\tau)M_1(\tau)+x^*(\tau)M_2(\tau))]\psi_I(0), \quad (3.5)$$

where T denotes the chronological product of the interaction-picture matrices given by Eq. (3.4). We investi-

gate first the case when the initial condition $\psi_I(0)$ is independent on the stochastic properties of the random variables x and x^*. In this case, in order to find the stochastic average (3.1) of Eq. (3.5), we have to compute the following functional integral:

$$\langle\psi_I(t)\rangle = \langle T\exp[i\int_0^t d\tau(x(\tau)M_1(\tau)+x^*(\tau)M_2(\tau))]\rangle\psi_I(0). \quad (3.6)$$

The functional integration in Eq. (3.6) can be done exactly by applying the formulas (2.3) and (2.4) for T-ordered J matrices[8]:

$$\langle\psi_I(t)\rangle = T\exp\left[-\tfrac{1}{2}\int_0^t d\tau_1\int_0^t d\tau_2(M_1(\tau_1),M_2(\tau_1)) \times\Delta(\tau_1\tau_2)\begin{pmatrix}M_1(\tau_1)\\M_2(\tau_2)\end{pmatrix}\right]\psi_I(0). \quad (3.7)$$

With the choice of the Δ functions for quasi-completely random process [see Eq. (2.8)] we obtain from Eq. (3.7) the following formula:

$$\langle\psi_I(t)\rangle = T\exp\left[-\tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\int_0^t d\tau\,\Gamma_{ij}^n\frac{d^nM_i(\tau)}{d\tau^n}\frac{d^nM_j(\tau)}{d\tau^n}\right]\psi_I(0). \quad (3.8)$$

This expression can be converted into a differential equation:

$$\frac{d}{dt}\langle\psi_I(t)\rangle = -\tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\Gamma_{ij}^n\frac{d^nM_i(t)}{dt^n}\frac{d^nM_j(t)}{dt^n}\langle\psi_I(t)\rangle. \quad (3.9)$$

The time derivatives of the $M_i(t)$ matrices can be expressed in terms of multicommutators. From Eq. (3.4) if follows that

$$\frac{d^nM_i(t)}{dt^n} = [[\cdots[M_i,M_0]\cdots M_0] = L^nM_i(t), \quad (3.10)$$

where L is the Liouville operator acting in the matrix M_1 or M_2 as follows:

$$L\circ = [\circ, M_0]. \quad (3.11)$$

From Eqs. (3.2) and (3.9) we obtain the following differential equation with constant coefficients for $\langle\psi\rangle$:

$$\frac{d\langle\psi(t)\rangle}{dt} = (M_0 - \tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\Gamma_{ij}^n(L^nM_i)(L^nM_j))\langle\psi(t)\rangle. \quad (3.12)$$

This equation is the main result of this paper. Solving this linear equation (for example, by Laplace transform technique) we obtain the exact solution of our problem. If $\Gamma_{ij}^n = 2D\delta_0^n(\delta_i^1\delta_j^2+\delta_i^2\delta_j^1)$, i.e., for a completely-random process Eq. (3.12) reduces to a result already obtained in the literature.

Equation (3.13) was obtained with an additional assumption that the initial condition does not depend on the random variables of the stochastic process.

We are going to generalize our results for the case when it is not so. We assume that the initial condition $\psi_I(0)$ has the following specific dependence on the random variables:

$$\psi_I(0) = \exp[i\int_{-\infty}^{\infty} ds\, g_1(s)x(s)+g_2(s)x^*(s)]\bar{\psi}_I(0), \quad (3.13)$$

where g_1 and g_2 are two arbitrary functions and $\bar{\psi}_I(0)$ is the remaining, statistically independent part of the initial condition. If we choose, for example, $g_1(s)=g_2(s)=\delta(s)$ we have a simple phase dependence of the initial condition on $x(0)$ and $x^*(0)$. This kind of dependence occurs in many atomic physics applications.[9] When the initial condition (3.13) is used we have the following modification of the formal solution (3.6):

$$\langle\psi_I(t)\rangle = \langle T\exp[i\int_{-\infty}^{\infty} d\tau((\theta(t-\tau)\theta(\tau)M_1(\tau)+g_1(\tau))x(\tau) + \theta(t-\tau)\theta(\tau)M_2(\tau)+g_2(\tau))x^*(\tau))]\bar{\psi}_I(0). \quad (3.14)$$

The functional integration in Eq. (3.14) can be done explicitly by applying Eqs. (2.3) and (2.4) with proper J and J^* functions:

$$\langle\psi_I(t)\rangle = T\exp[-\tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\Gamma_{ij}^n \times\int_{-\infty}^{\infty} ds((\theta(t-s)\theta(s)\frac{d^nM_i(s)}{ds^n}\frac{d^ng_j}{ds^n}) + (\theta(t-s)\theta(s)\frac{d^nM_i}{ds^n}+\frac{d^ng_j}{ds^n})\Big)\Big]\bar{\psi}_I(0). \quad (3.15)$$

We can convert this expression into the following differential equation:

$$\frac{d\langle\psi_I(t)\rangle}{dt} = -\tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\Gamma_{ij}^n\Big(\frac{d^nM_i(t)}{dt^n}\frac{d^nM_j(t)}{dt^n}+\frac{d^ng_i}{dt^n}\frac{d^nM_j(t)}{dt^n} + \frac{d^nM_i(t)}{dt}\frac{d^ng_j}{dt}\Big)\langle\psi_I(t)\rangle. \quad (3.16)$$

Using the relation (3.2) and (3.10) we rewrite this equation in the following form:

$$\frac{d\langle\psi\rangle}{dt} = (M_0 - \tfrac{1}{2}\sum_{n=0}^{N}\sum_{ij}\Gamma_{ij}^n(L^nM_i)(L^nM_j)+\frac{d^ng_i(t)}{dt^n}(L^nM_j) + \frac{d^ng_j}{dt^n}(L^nM_i))\langle\psi\rangle. \quad (3.17)$$

For completely random processes with $\Gamma_{ij}^n = 2D\delta_0^n(\delta_i^1\delta_j^2+\delta_i^2\delta_j^1)$ we obtain from Eq. (3.17)

$$\frac{d\langle\psi\rangle}{dt} = (M_0 - DM_1M_2 - DM_2M_1 - Dg_1(t)M_2 - Dg_2(t)M_1)\langle\psi\rangle. \quad (3.18)$$

The phase of the initial condition (3.13) enters the differential equation (3.18) in the form of time-dependent coefficients $g_1(t)$ and $g_2(t)$. Equation (3.17) is a generalization of the result (3.12) for statistically dependent initial condition (3.13).

IV. EXAMPLE OF AN EXACTLY SOLUBLE MSP

As an example of an exactly soluble multiplicative stochastic process let us take a well-known model—Hamiltonian from nonlinear optics[10]:

$$H = \hbar\omega_0 b^*b + \tfrac{1}{2}(b^{*2}\mathcal{E}+\mathcal{E}^*b^2). \quad (4.1)$$

This Hamiltonian describes generation of higher harmonics by a quantum oscillator coupled to a classical

electromagnetic field. In order to have a stochastic process we assume that the electromagnetic field beside its optical frequency ω has a real stochastic phase. The electromagnetic field amplitude has then the following form:

$$\mathcal{E}(t)=\mathcal{E}_0 \exp[-i\omega t - i\int_0^t ds\, x(s)], \tag{4.2}$$

where $x(s)$ is a real random variable with a Gaussian statistic:

$$\langle x(s)x(t)\rangle = 2D\delta(t-s). \tag{4.3}$$

The Hamiltonian (4.1) leads to the following Heisenberg equation of motion:

$$\frac{db}{dt} = i\omega_0 b - i\mathcal{E}(t)b^*. \tag{4.4}$$

Equation (4.4) has the form of a multiplicative stochastic process illustrated by the example (1.2) in the introduction. The Heisenberg equations of motion generated by the Hamiltonian (4.1) can be written in the form of the matrix equation (1.3) with

$$\psi(t) = (b(t),\ \exp[-i\omega t - i\int_0^t x(s)ds]b^*(t)), \tag{4.5a}$$

$$M_0 = \begin{bmatrix} -i\omega_0 & -i\mathcal{E}_0 \\ i\mathcal{E}_0^* & i(\omega_0-\omega) \end{bmatrix}, \tag{4.5b}$$

$$M_1 = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix},\quad M_2 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \tag{4.5c}$$

According to the theory developed in this paper the stochastic average satisfies the following differential equation:

$$\frac{d\langle\psi\rangle}{dt} = (M_0 - DM_1^2)\langle\psi\rangle. \tag{4.6}$$

This equation can be solved using the Laplace transform technique. After simple calculations we obtain

$$\langle b(t)\rangle = \int_C \frac{dz}{2\pi i} \times e^{zt}\, \frac{b(0)(z-i\omega_0+i\omega+D) - i\mathcal{E}_0 b^*(0)}{z^2 + z(D+i\omega) + \omega_0^2 - \omega\omega_0 + i\omega_0 D - \mathcal{E}_0\mathcal{E}_0^*}. \tag{4.7}$$

Computing the roots of the algebraic equation in the denominator in Eq. (4.7) and choosing properly the contour of integration C we find the explicit time evolution of $\langle\psi(t)\rangle$. The solution (4.7) is a simple example of an exact solution of a multiplicative stochastic process and a straightforward application of the method.

V. CONCLUSIONS

In this paper we have presented a method of how to solve exactly operator-valid equations with stochastic coefficients. For completely random Gaussian processes we recover the result already published in the literature.[2] The Feynman path formulation of Gaussian processes simplify greatly the previous proof removing unnecessary assumptions. For quasicompletely random processes and statistically dependent initial conditions new solutions are obtained. Physical applications of multiplicative stochastic processes in atomic physics will be published separately.[9]

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Variational formalism for spinning particles

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We relate here the geometric formulation of Hamilton's principle presented in our previous paper to the usual one in terms of a Lagrangian function. The exact conditions for their equivalence are obtained and a method is given for the construction of a Lagrangian function. The formalism is extended to spinning particles and a local Lagrangian is constructed in this case also. However, this function cannot be extended to a global one.

1. INTRODUCTION

In our previous paper[1] we presented a geometrical framework which made it possible for us to treat Hamilton's Principle in a coordinate-free manner.

A mechanical system was characterized by its evolution space, E, and Lagrange form, σ. The equations of motion are expressed as

$$\frac{d}{dt}(\tilde{g})(t) \in \operatorname{Ker} \sigma_{\tilde{g}(t)}, \tag{1.1}$$

where $\tilde{g}$ denotes the lift to E of the motion-curve g lying in configuration space, Q.

In the classical case, when a Lagrangian function L is given, one can introduce a λ field of 1-forms called the system's *Cartan form*, in terms of which the Euler–Lagrange equations take the form

$$\frac{d}{dt}(\tilde{g})(t) \in \operatorname{Ker} d\lambda_{\tilde{g}(t)}. \tag{1.2}$$

Comparing (1.1) and (1.2) we said that a system given by (E, σ) has a local variational description if there exists at least locally (i.e., defined on a local chart) a λ field of 1-forms for which $\sigma = d\lambda$.

The necessary and sufficient condition for the existence of such a λ is $d\sigma = 0$, referred to by Souriau[2] as Maxwell's Principle.

Our most interesting result was to prove that although the equations of motion of spinning particles can be expressed in terms of a Lagrange form σ,[1] satisfying $d\sigma = 0$, there cannot exist a globally defined λ with $d\lambda = \sigma$.

However, the definition of the Cartan form given in Ref. 1 was rather "*ad hoc*" and valid only in the classical case. Also, it was not entirely clear what the above result meant in terms of a Lagrangian function.

We propose here a slightly different framework which can easily be extended to include spinning particles as well.

We shall study the world lines in $Q \times R$; the role of the evolution space will be played by a subset F of $T(Q \times R)$. L will be substituted by a homogenized Lagrangian, $\mathcal{L}$. Then we can state that there is a unique way to geometrize the problem, namely by using the field of 1-forms $\Lambda = \dot{d}\mathcal{L}$. ($\dot{d}$ denotes the operation of "vertical differentiation," see Klein[3,4] or Godbillon.[5]) This Λ can be projected onto E; its image λ coincides with the Cartan form introduced in Ref. 1. Using Klein's results we can establish the necessary and sufficient conditions for the possibility to recover a Lagrangian function from a field of 1-forms λ defined on the evolution space. In local coordinates this is expressed as λ must be of the form $a_\alpha\, dq^\alpha + b\, dt$ $(\alpha = 1, \ldots, n)$ and

$$v^\alpha \partial_\beta a_\alpha + \partial_\beta b = 0, \quad \beta = 1, \ldots, n \tag{1.3}$$

must hold. In this case L has the local form,

$$L(q, v, t) = a_\alpha v^\alpha + b. \tag{1.4}$$

In this framework the generalized solutions of the variational problem will be constant-dimensional submanifolds of F called evolution leaves. Their projections on space–time are C^∞ curves satisfying the Lagrange equations. These leaves can be set in one-to-one correspondence with the evolution curves of E.

Hence our results obtained in Ref. 1 really mean that there cannot exist any globally defined Lagrangian function for the spinning particle; nevertheless, condition (1.3) is satisfied and we can construct a local Lagrangian function in this case as well.

2. GENERAL THEORY

We give here a short outline of a geometrical framework slightly differing from that presented in Ref. 1. This is a kind of synthesis of the ideas of Souriau[2] and Klein.[3,4]

The basic point is to work with world lines in $Q \times R$ rather than with motion in configuration space, Q, time being a fixed exterior parameter. This approach is natural in relativity and turns out to be useful in this context as well. Now we carry over our entire apparatus to this context.

A. Motions

To the motions in Q correspond the world lines parametrized by an arbitrary parameter τ. In local coordinates a world line is

$$h : \tau \to h(\tau) = (g(\tau), t(\tau)) \in Q \times R. \tag{2.1}$$

It is required that $\dot{t} > 0$ (the dot denotes the derivative of t by τ).

B. The Hamiltonian action

A change in parametrization shows that the Hamiltonian action has the form

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$$\vartheta(g)=\int_{\tau_1}^{\tau_2} L\left(g(\tau),\frac{\dot g(\tau)}{\dot t(\tau)},t(\tau)\right)\ \dot t(\tau)\,d\tau. \tag{2.2}$$

If $x=(q,t)$ is a local chart for $Q\times R$, then the corresponding natural chart of $T(Q\times R)$ will be denoted by $(x,\dot x)=(q,t,\dot q,\dot t)$.

Define $F:=\{(x,\dot x)\in T(Q\times R):\dot t>0\}$ and introduce the *homogenized Lagrangian* $\mathcal{L}$ as:

$$\mathcal{L}:F\ni(q,t,\dot q,\dot t)\to L\left(q,\frac{\dot q}{\dot t},t\right)\dot t. \tag{2.3}$$

$\mathcal{L}$ is homogenous of order 1 in $\dot x$; using $\mathcal{L}$ the Hamiltonian action is

$$\vartheta(g)=\int_{\tau_1}^{\tau_2}\mathcal{L}(h,\dot h)\,d\tau. \tag{2.4}$$

C. States

In Ref. 1 we have identified the states of the system with the points of E. The points of F can be thought of as states as well; two points of F represent the same state and hence are called physically equivalent if their first coordinates coincide and second coordinates are proportional.

Define

$$\Pi:F\to E \text{ as } \Pi(q,t,\dot q,\dot t)=\left(q,\frac{\dot q}{\dot t},t\right),$$

then two points of F are physically equivalent if they are mapped to the same points of E by Π.

Let h be a curve in $Q\times R$ parametrized by τ. Then define

$$\tilde h^{\tau}(\tau):=(h(\tau),\dot h(\tau)) \tag{2.5}$$

to be the lift of h to F according to τ. By changing the parameter we get an entire family of curves in F, which cover a two-dimensional submanifold lying in F. In particular, to the motion curves corresponds a system of two-dimensional submanifolds with the property that through every point of F passes exactly one such submanifold called an *evolution leaf*. Π sets up a one-to-one correspondence between these leaves and the evolution curves of E. Hence the system's evolution can be described alternatively by the evolution leaves of F.

D. The Cartan form

The "geometrization" of the problem—which turned out to be useful in Ref. 1—is based on the following lemma:

Lemma: Let there be given an $\mathcal{L}:F\to R$ function which is homogenous of order 1 in $\dot x$. Then there exists a unique field of 1-forms Λ of F which satisfies

$$\int_{\tau_1}^{\tau_2}\mathcal{L}(h(\tau),\dot h(\tau))\,d\tau=\int_{\tilde h^{\tau}}\Lambda. \tag{2.6}$$

In local coordinates this Λ is given as

$$\Lambda=\dot d\mathcal{L}=\partial_{\alpha}^{\cdot}\mathcal{L}\,dx^{\alpha}, \tag{2.7}$$

the "vertical derivative" of $\mathcal{L}$. (For the definition of $\dot d$ see Klein,[3,4] or Godbillon[5]; $\partial_{\alpha}^{\cdot}\mathcal{L}$ denotes $\partial\mathcal{L}/\partial\dot x^{\alpha}$.)

One verifies at once that Λ is homogeneous of order 0, semibasic, and $\dot d$-closed, i.e., $\dot d\Lambda=0$. Klein has shown in Ref. 3 that these conditions are also sufficient for Λ to be locally, i.e., on a local chart, of the form $\dot d\mathcal{L}$. In local coordinates, if Λ is given as

$$\Lambda=A_{\alpha}dx^{\alpha},\quad \text{then } \mathcal{L}=A_{\alpha}\dot x^{\alpha}. \tag{2.8}$$

The above defined Λ can easily be related to the Cartan form λ introduced in Ref. 1.

Definition: An α p-form on F is said to be projectable onto E iff there exists a unique β p-form on E for which $\alpha=\Pi^*(\beta)$.

One shows that a semibasic 1-form on F is projectable if it is homogenous of order 0; consequently our Λ defined in (2.7) is projectable.

In local coordinates we get

$$\Lambda=\left(\frac{\partial L}{\partial v^{\alpha}}\cdot\Pi\right)dq^{\alpha}+\left[\left(L-\frac{\dot q}{\dot t}\frac{\partial L}{\partial v^{\alpha}}\right)\cdot\Pi\right]dt. \tag{2.9}$$

Thus its image under Π is exactly λ, the Cartan form introduced in Ref. 1. Conversely, if we are given a λ field of 1-forms on E, we can pull it back to F. If $\lambda=a_{\alpha}dq^{\alpha}+b\,dt$ is a semibasic 1-form on E, then its pullback is

$$\Pi^*(\lambda)=(a_{\alpha}\cdot\Pi)dq^{\alpha}+(b\cdot\Pi)dt \tag{2.10}$$

One verifies that $\dot d(\Pi^*(\lambda))=0$ iff

$$v^{\alpha}\partial_{\beta}^{\cdot}a_{\alpha}+\partial_{\beta}^{\cdot}b=0,\quad \beta=1,\dots,n. \tag{2.11}$$

In this case the local Lagrangian function is given as

$$L(q,v,t)=a_{\alpha}v^{\alpha}+b. \tag{2.12}$$

These last two formulas will be very important, for they not only express the necessary and sufficient conditions under which a local Lagrangian function can be recovered, but they even give its explicit form.

E. Calculus of variations

Our investigations in Ref. 1 were based on the heuristic idea that calculus of variations can be thought of as a differential calculus on an infinite-dimensional manifold. We will also keep in mind this idea now; the geometrical framework will be slightly different.

Let us choose two points in space—time, $x_1=(q_1,t_1)$ and $x_2=(q_2,t_2)$ and consider the C^{∞} curves joining these points. (Denote their set again by P.) The manifold structure on P is defined by introducing a Banach-space structure on its tangent space. One of the basic postulates of classical mechanics is the absolute status of time; this property will be reflected by the requirement that time be not varied. Hence we define the tangent space of P at a curve h to be the set of all C^{∞} vector fields along h which can be extended onto a neighborhood of h, vanish at the endpoints and have zero time-component, i.e., have the local form $(Y_q,0)$.[6]

In order to calculate the stationary curves a very similar treatment as in Ref. 1 is applied. Finally we get: The directional derivative of ϑ by an element Y of the tangent space at a point g,

$$Y(\vartheta)(g)=\int_{\tilde h^{\tau}}d\Lambda(\cdot\,,\tilde Y), \tag{2.13}$$

where $\tilde Y$ again denotes the lifting of the vector field Y to F; in local coordinates

$$\tilde{Y}=(Y,\dot{Y}) \quad \text{with } \dot{Y}^{\alpha}=\partial_{\beta}Y^{\beta}\dot{X}^{\alpha} \tag{2.14}$$

(see Klein[3]).

Now, the corresponding form of the Du Bois–Reymond lemma assures that

$$Y(\mathcal{G})(g)=0 \text{ iff } d\Lambda(\tilde{\dot{h}},\tilde{Y})=0, \ \underset{\approx}{\forall} \ Y\in T_h P. \tag{2.15}$$

Note that because time is not varied, this does not mean that $\dot{\tilde{h}}^{\tau}(\tau)\in \operatorname{Ker} d\Lambda_{\tilde{h}^{\tau}(\tau)}$, nevertheless a similar line of thought as in Ref. 1 can be applied:

$$H_y:=\{X\in T_yT(Q_xR): d\Lambda(X,Y)=0, \ \underset{\approx}{\forall} \ Y\in T_yT(Q\times R)$$

of the form $(Y_q^{\cdot}0, Y_q^{\cdot}, 0)\}$.[6] (2.16)

Then one verifies that g is a stationary curve if

$$\dot{\tilde{h}}^{\tau}(\tau)\in H_{h(\tau)} \tag{2.17}$$

$[h(\tau)=(g(\tau),t(\tau))]$.

Suppose H_y has constant dimension for every $y\in F$; one verifies then that if $X, Y\in H_y$, then their Lie bracket, $[X,Z]$ belongs also to H_y; hence we can apply the corresponding theorem of fiber spaces (see Souriau[2]) and get:

Proposition: Through every point of F passes exactly one leaf, whose tangent space coincides there with the H-subspace ordered to this point : We call these leaves the leaves belonging to Λ (or $d\Lambda$).

One can verify that if we start with L, then codim H_y is equal to the rank of the matrix $\|\partial_{\dot{\alpha}\dot{\beta}}L\|$; the problem will be said to be a regular one if this rank is n; the leaves are then two-dimensional submanifolds of F. We shall consider them as the generalized solutions of the variational problem. By a straightforward calculation one verifies that:

Theorem: Suppose the problem is regular; then the leaves belonging to $d\dot{d}\dot{L}$ have the following property: Their projections onto $Q\times R$ are C^{∞}-curves satisfying the Lagrange equations.

F. Relation to symplectic mechanics

We see that the 2-form $d\dot{d}\dot{L}$ plays a fundamental role similar to that of σ in Ref. 1. This is a consequence of the following.

Proposition: $\Sigma:=d\dot{d}\dot{L}$ can be projected onto E and $d\Sigma=0$, $\dot{d}\Sigma=0$.

If $\Lambda=\Pi^{*}(\lambda)$, then $\Sigma=\Pi^{*}(d\lambda)$.

The fundamental result of Klein in Ref. 4 states that if Σ can be projected on E, and $d\Sigma=0$, $\dot{d}\Sigma=0$ both are valid, then there exists a local L with $\Sigma=d\dot{d}\dot{L}$. The most general L is given as $L\to kL+\partial_{\alpha}f\dot{x}^{\alpha}$ where f is a function on $Q\times R$ alone. (Here we recognize the well-known gauge transformation.) In terms of L this means,

$$L\to kL+\frac{\partial f}{\partial q^{\alpha}}v^{\alpha}+\frac{\partial f}{\partial t}.$$

Conversely, if we are given a pair (E,σ), we may pull σ back to F and so define a Σ; $d\sigma=0$ iff $d\Sigma=0$. Our local variational principle proposed in Ref. 1 states the existence of a locally defined λ with $d\lambda=\sigma$; as we have just seen, this does not mean automatically the existence of a Lagrangian function. In order to decide whether this stronger requirement has to be made or not, we have to study spinning particles, for in classical cases the problem is solved.

3. VARIATIONAL FORMALISM FOR SPINNING PARTICLES

After this general framework we are ready to turn to the construction of a variational formalism for spinning particles. Remember, that in this case $E=T(Q)\times R\times S^2$, and the Lagrange form is given as

$$\sigma=\{(mdv-E\,dt)\wedge(dq-vdt)+\langle F, dq\times dq\rangle\}$$
$$+\{d(\mu\langle s,B\rangle dt)-\lambda\langle s, ds\times ds\rangle,\} \tag{3.1}$$

($\langle\cdot,\cdot\rangle$ represents the scalar product in 3-space). Here the first curly bracket is the Lagrange form of a particle moving in an electromagnetic field; in what follows we shall study only the second one representing the spin interaction.

As spin can be thought of as an inner degree of freedom, it seems to be natural to treat it together with configuration space; we will simply substitute Q by $Q\times S^2$. A local Lagrangian function would then be an L defined on a local chart of $T(Q\times S^2)\times R$. To L would correspond a homogenized $\mathcal{L}$ according to the formula

$$\mathcal{L}(q,s,t,\dot{q},\dot{s},\dot{t}):=L\left(q,s,\frac{\dot{q}}{\dot{t}},\frac{\dot{s}}{\dot{t}},t\right)\dot{t}, \tag{3.2}$$

which yields the Cartan form

$$\Lambda=\frac{\partial\mathcal{L}}{\partial\dot{q}^{\alpha}}dq^{\alpha}+\frac{\partial\mathcal{L}}{\partial\dot{t}}dt+\frac{\partial\mathcal{L}}{\partial\dot{s}^{\alpha}}ds^{\alpha}. \tag{3.3}$$

The exterior derivative of this must coincide with the pullback to F of the system's Lagrange form. The evolution space would be $T(Q\times S^2)\times R$. Our original E was merely $T(Q)\times R\times S^2$, but this does not matter as σ can be trivially extended to $T(Q\times S^2)\times R$ as it has no $d\dot{s}$ component.

In order to find a variational formalism for spinning particles we have only to find an additional term of the spin part of σ, σ_{spin}.

The pullback of the spin part to F is simply

$$\Pi^{*}(\sigma_{\text{spin}})=d(\mu\langle s,b\rangle dt)-\lambda\langle s, ds\times ds\rangle, \tag{3.4}$$

where λs is the proper angular momentum, μs is the proper magnetic momentum (see Ref. 1 or 2) and λ, μ are real constants.

Thus we have to solve the equation

$$d\dot{d}\dot{\mathcal{L}}_{\text{spin}}=\Pi^{*}(\sigma_{\text{spin}}). \tag{3.5}$$

Our most interesting result in Ref. 1 was that there cannot exist a globally defined Θ field of 1-forms with $d\Theta=\sigma_{\text{spin}}$; (3.5) shows then that this really means that no global Lagrangian function can exist. In order to construct a local Lagrangian we must find first a local potential for the spin part of σ. The magnetic-field spin-interaction part is itself a total differential, hence

a (global) potential for it is

$$\lambda^{(1)}_{\text{spin}} = \mu\langle s, B\rangle dt. \tag{3.6}$$

Let us study now the second term. We introduce the atlas of S^2 consisting of the charts F_+ and $F_-: R^2 \to S^2$:

$$[F_\pm(s)]^\alpha = \frac{2s^\alpha}{1+|s|^2},\ \alpha = 1,2, \quad s = (s^1, s^2),$$

$$[F_\pm s^3] = \pm\frac{1-|s|^2}{1+|s|^2}. \tag{3.7}$$

One verifies at once that on these charts the form

$$\lambda^{(2)}_{\text{spin}} = \pm 2\lambda \frac{s^1 ds^2 - s^2 ds^1}{1+(s^1)^2+(s^2)^2} \tag{3.8}$$

is a potential for $\sigma^{(2)}_{\text{spin}}$. The results of (2.4) can be then applied; (2.11) is verified, hence by (2.12) the corresponding local Lagrangian functions are

$$L^{(1)}_{\text{spin}}(s, \dot{s}) = \mu\langle s, B\rangle, \tag{3.9}$$

$$L^{(2)}_{\text{spin}}(s, \dot{s}) = \pm\frac{2\lambda}{1+|s|^2}[-s^2\dot{s}^1 + s^1\dot{s}^2]. \tag{3.10}$$

Summing up, the local Lagrangian function for spinning particles is given in the above coordinates as

$$L_\pm(q, s, v, \dot{s}, t) = \left\{\tfrac{1}{2}[mv^2 + \langle A, q\rangle] - v(q)\right\} + \left\{\mu\langle s, B\rangle \pm \frac{2\lambda}{1+|s|^2}[-s^2\dot{s}^1 + s^1\dot{s}^2]\right\}, \tag{3.11}$$

with gauge transformation

$$L \to kL + \frac{\partial f}{\partial q^\alpha} v^\alpha + \frac{\partial f}{\partial t} + \frac{\partial f}{\partial s^\alpha}\dot{s}^\alpha.$$

(Here f is any real function on $Q\times S^2\times R$.)

From (3.10) we see at once that none of these local Lagrangians can be extended onto the entire evolution space. This can be demonstrated by observing that:

$$s_1 = 0, \quad s_2 \to \infty, \quad \dot{s}_1 = s_2, \quad \dot{s}_2 = 0,$$

$$s_1 = 0, \quad s_2 \to \infty, \quad \dot{s}_1 = 0, \quad \dot{s}_2 = 0,$$

both tend to the same point of TS^2 [namely to the 0-tangent vector at the lower (resp. upper) pole], but L tends in the first case to $\mp 2\lambda$, in the second case to 0. Hence L cannot have a limit.

In this case the rank of $|\partial_{\dot{a}\dot{b}} L|$ is $2n+2$, H_y is four-dimensional; the leaves belonging to L are thus four-dimensional submanifolds of $T(Q\times S^2\times R)$. Their projections onto $Q\times S^2\times R$ are C^∞ curves satisfying the Thomas equations. (See Refs. 1 and 2.)

4. CONCLUSION

We have shown that even the spinning particle has a local Lagrangian function. Thus we are led to the following modification of our local variational principle:

Definition: A mechanical system given by (E, σ) is said to have a local *variational description* if there exists a λ field of 1-forms with the following properties:

(i) $d\lambda = \sigma$

(ii) λ is semibasic,

(iii) the pullback of λ to F is $\dot{d}$-closed, $\dot{d}(\Pi^*(\lambda) = 0$.

Under these conditions there exists a Lagrangian function L on each local chart of E and the system's Lagrange form is the projection of $d\dot{d}L$ onto E.

The necessary and sufficient condition for (E, σ) to have a local variational description is

(i) $d\sigma = 0$ (Maxwell's principle),

(ii) $\dot{d}(\Pi^*\sigma) = 0$.

The *local variational principle* states that these conditions are verified for any mechanical system.

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[6] *Note added in proof*: It can be shown that in the case under consideration one can allow more general variations of the form (Y_q, Y_t). Equation (2.16) becomes then

$$H_y = \operatorname{Ker} d_{\wedge\tilde{h}^\tau(\tau)},$$

and (2.17) will be

$$\dot{\tilde{h}}^\tau(\tau) \subset \operatorname{Ker} d_{\wedge\tilde{h}^\tau(\sigma)},$$

see, for instance, P. Horváthy, thesis, 1978 (in Hungarian).

Nonlinear approach to inverse scattering

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The inverse scattering problem for the scalar wave equation associated with propagation through a medium whose index of refraction differs from that of free space in a region of compact support is treated when the scattered data is given for diverse directions of (plane wave) incidence, scattered directions, and frequencies. The problem is formulated in terms of the minimization of a nonlinear functional which is bounded below, subject to constraints. It is shown that the conditional-gradient method may be employed, the iteration process converging to stationary points. The linearized version (corresponding to the perturbed wave equation with only the linear perturbed terms retained) of the nonlinear functional is considered as a special case. In particular the linearized version related to the Born approximation leads to some additional new results.

I. INTRODUCTION

The inverse scattering problem for the scalar wave equation associated with propagation through a medium whose index of refraction differs from that of free space in a region of compact support is treated when the scattered data is given for diverse directions of (plane wave) incidence, scattered directions, and frequencies. Included in the analysis are errors in the measured data.

As a preliminary the results of the direct scattering process is presented. Then the inverse problem is formulated in terms of minimizing a nonlinear functional which is bounded below, subject to constraints. It is shown that the conditional-gradient methode may be employed, the iteration process converging to stationary points.

The linearized version (corresponding to the perturbed wave equation with only the linear perturbed terms retained) of the nonlinear functional is considered as a special case. It is shown that this simplified model corresponds to known techniques. In particular, the linearized version corresponding to the Born approximation is treated in some detail, leading to some additional new results.

THE DIRECT SCATTERING PROBLEM

Consider the equation

$$\Delta u + k^2 n^2(\mathbf{x}) u = 0, \quad \mathbf{x} \text{ in } \mathbb{R}^3 \tag{1}$$

where the index of refraction $n(\mathbf{x})$ has the property that it is a real continuous function which is identically equal to unity outside some sphere of finite radius. Here, $k = \omega/c$ is the wavenumber associated with the suppressed harmonic time dependence of the form $\exp(-i\omega t)$.

Consider an incident wave

$$u^i(\mathbf{x}) = \exp(i\,\mathbf{k}^i \cdot \mathbf{x})$$

where the incident propagation vector

$$\mathbf{k}^i = k\,(\sin\theta^i\cos\varphi^i\mathbf{i} + \sin\theta^i\sin\varphi^i\mathbf{j} + \cos\theta^i\mathbf{k})$$

is in the direction given by the angular variables (θ^i, φ^i) of the spherical polar coordinate system. The presence of the scattering object represented by the non-vanishing of $(n^2 - 1)$, produces a scattered field $u^s(\mathbf{x})$. With the decomposition

$$u(\mathbf{x}) = u^i(\mathbf{x}) + u^s(\mathbf{x}).$$

Equation (1) can be placed in the form

$$\Delta u^s + k^2 n^2(\mathbf{x}) u^s = k^2[1 - n^2(\mathbf{x})] u^i(\mathbf{x}). \tag{2}$$

The following result is obtained from Ref. 1.

Theorem: When $[n^2(\mathbf{x}) - 1]$ is a real continuous function of compact support, the unique C^2 solution $u^s(\mathbf{x})$ of Eq. (2) exists satisfying the radiation condition as $|x| = r \to \infty$

$$\frac{\partial u^s}{\partial r} = iku^s + o\left(\frac{1}{r}\right).$$

For further analysis Eq. (2) will be converted to an integral equation. As a preliminary to this, set

$$v(\mathbf{x}) = n^2(\mathbf{x}) - 1. \tag{3}$$

it will be assumed henceforth that the support of $v(\mathbf{x})$ is contained in a fixed domain D_0, where D_0 is a ball of radius R_0. Let D be a ball of radius R_1 containing D_0 so that $R_1 > R_0$. A fixed auxiliary function $\eta(\mathbf{x})$ will then be defined that has the properties,

(1) $\eta(\mathbf{x})$ is a real Holder-differentiable function,

(2) $\eta(\mathbf{x}) \equiv 0$ for $|\mathbf{x}| > R_1$,

(3) $\eta(\mathbf{x}) \equiv 1$, for $\mathbf{x} \in D_0$.

Equation (2) is then placed in the form

$$u(\mathbf{x}) = u^i(\mathbf{x}) + \frac{k^2}{4\pi}\int_D \frac{\exp(ik|\mathbf{x} - \mathbf{y}|)}{|\mathbf{x} - \mathbf{y}|}\, v(\mathbf{y})\eta(\mathbf{y})u(\mathbf{y})\,d\mathbf{y}, \tag{4}$$

The reason for the introduction of $\eta(\mathbf{x})$ into the integral equation will become apparent below.

When $|\mathbf{x}| \to \infty$, the far field behavior is given by

$$u^s(\mathbf{x}) \sim \frac{\exp(ik|\mathbf{x}|)}{|\mathbf{x}|} g(\mathbf{k}^i, \mathbf{k}^s; v), \quad \mathbf{k}^s = \frac{k\mathbf{x}}{|\mathbf{x}|}$$

where the complex scattering amplitude $g(\mathbf{k}^i, \mathbf{k}^s; v)$ has the form

$$g(\mathbf{k}^i, \mathbf{k}^s; v) = \frac{k^2}{4\pi}\int_D \exp(-i\mathbf{k}^s \cdot \mathbf{y}) v(\mathbf{y})\eta(\mathbf{y})u(\mathbf{y})\,d\mathbf{y} \tag{5}$$

$\mathbf{k}^s$ is a vector of length k in the scattered direction represented by the angular variables (θ^s, φ^s), i.e.;

$$\mathbf{k}^s = k[\sin\theta^s\cos\varphi^s\mathbf{i} + \sin\theta^s\sin\varphi^s\mathbf{j} + \cos\theta^s\mathbf{k}\,].$$

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FORMULATION OF THE INVERSE PROBLEM

The inverse problem consists of determining $v(\mathbf{x})$ hence $n(\mathbf{x})$ given the scattered field data. When measurements are made in the far field, values of $g(\mathbf{k}^i,\mathbf{k}^s;v)$ are given for a set of incident directions $\mathbf{k}^i$, scattered directions $\mathbf{k}^s$ observed either at a single frequency as denoted by a single wave number k, or at a set of different frequencies.

In what follows, the actual material properties of the scatterer will be denoted by $n^*(\mathbf{x})$ or $v^*(\mathbf{x})$. As mentioned previously, the support of $v^*(\mathbf{x})$ will be contained in D_0. The scattering amplitude of the scatterer will be denoted by $g(\mathbf{k}^i,\mathbf{k}^s;v^*)$. The measured far scattered field for a particular direction of incidence $\mathbf{k}^i$, scattered direction $\mathbf{k}^s$, and wavenumber $k=|\mathbf{k}^i|=|\mathbf{k}^s|$ will have the form

$$g^\epsilon(\mathbf{k}^i,\mathbf{k}^s;v^*)=g(\mathbf{k}^i,\mathbf{k}^s;v^*)+\epsilon(\mathbf{k}^i,\mathbf{k}^s) \tag{6}$$

Where $\epsilon(\mathbf{k}^i,\mathbf{k}^s)$ denotes the errors of measurement in the scattered field.

If the measurements of the scattered far field consist of a set of N discrete measurements made in the scattering directions $\mathbf{k}_l^s$, $l=1,2,\ldots,N$, corresponding to the directions of incidence $\mathbf{k}_l^i$ with $|\mathbf{k}_l^i|=|\mathbf{k}_l^s|$, one can form the following nonlinear functional:

$$f(v)=\sum_{l=1}^{N} W(\mathbf{k}_l^i,\mathbf{k}_l^s)\left|g(\mathbf{k}_l^i,\mathbf{k}_l^s;v)-g^\epsilon(\mathbf{k}_l^i,\mathbf{k}_l^s;v^*)\right|^2. \tag{7}$$

Here $W(\mathbf{k}^i,\mathbf{k}^s)$ is a nonnegative weight function depending upon $\mathbf{k}^i$ and $\mathbf{k}^s$ only, and is assigned *a priori*. It can be chosen to place greater weight on those measurements that have the least error. The optimum choice of $W(\mathbf{k}^i,\mathbf{k}^s)$ will not be investigated here. However, a particular choice for the weight function will be given below in the section on the Born approximation.

If there are no errors in the measurement, it is seen that $f(v)=0$ when $v=v^*$. The effect of errors may do two things, change the value of the minimum [the local minimum of $f(v)$ may no longer be zero], and change the position of the minimum corresponding to v^* to a perturbed value v_ϵ^*.

In the presence of errors in the data, as is obvious, one cannot hope to obtain v^* precisely, but must settle for a suitable approximation. Such an approximation is given by v_ϵ^*, and since as will be shown later, the derivative of $f(v)$ is bounded on a suitable set, v_ϵ^* will be close to v^* when the errors are sufficiently small. Thus v^* or its approximation in the presence of errors in the data, v_ϵ^* will be sought. (In subsequent analysis, the subscript ϵ will be suppressed.)

Since $f(v)$ is a nonnegative functional, the mathematical problem reduces to finding the value or values of v which minimizes $f(v)$.

Note that the measurements do not have to be made at the same frequency. Since one can allow $|\mathbf{k}_l^s|\neq|\mathbf{k}_m^s|$ for $l\neq m$. However, if they all are at the same frequency, then $|\mathbf{k}_l^s|=k$, $l=1,2,\ldots,N$.

If the far field data consists of measurements in the cone K^s $(0\leq\theta^s\leq\theta_0,\ 0\leq\varphi^s\leq 2\pi)$ of scattered directions corresponding to a single direction of incidence and frequency, then the nonlinear function has the form

$$f(v,\mathbf{k}^i)=\int_{K^s} W(\mathbf{k}^i,\mathbf{k}^s)\left|g(\mathbf{k}^i,\mathbf{k}^s;v)-g^\epsilon(\mathbf{k}^i,\mathbf{k}^s;v^*)\right|^2 d\Omega^s \tag{8a}$$

where $d\Omega^s=\sin\theta^s\,d\theta^s d\varphi^s$ is the element of solid angle in the scattered direction.

If, at the same time, the measurements are made over a cone K^i of incident directions (θ^i,φ^i) but still a single frequency, then

$$f(v)=\int_{K_i} f(v,\mathbf{k}^i)\,d\Omega^i \tag{8b}$$

where $d\Omega^i=\sin\theta^i d\theta^i d\varphi^i$

As pointed out by Wolf,[2] such measurements can be made in the near field of the scatterer. In particular if the direction of the incident wave is in the positive x_3 or $\theta^i=0$ direction, the scattered field measurements over the hemisphere $0\leq\theta^s<\pi/2$, $0\leq\varphi^s\leq 2\pi$, can be obtained from near field measurements over the plane $x_3=d$ where the region D or the scatterer lies in the half-space $x_3<d$. This result is obtained by use of the plane wave expansion

$$\frac{\exp(ik|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}=\frac{ik}{2\pi}\times\iint_{-\infty}^{\infty}\exp\{ik[p(x_1-y_1)+q(x_2-y_2)+(1-p^2-q^2)^{1/2}|x_3-y_3|]\}[(1-p^2-q^2)]^{-1/2}\times dp\,dq$$

where $(1-p^2-q^2)^{1/2}=i(p^2-q^2-1)^{1/2}$ if $p^2+q^2>1$. When this is substituted into Eq. (4), the scattered field on the plane $x_3=d$ has the form

$$u^s(\mathbf{x})=\frac{ik}{2\pi}\times\iint_{-\infty}^{\infty}\frac{\exp\{ik[px_1+qx_2+(1-p^2-q^2)^{1/2}x_3]A(p,q)\}}{(1-p^2-q^2)^{1/2}}dp\,dq,$$

where

$$A(p,q)=\frac{k^2}{4\pi}\int_D\exp[-ik(py_1+qy_2+(1-p^2-q^2)^{1/2}y_3)]\times v(\mathbf{y})\eta(\mathbf{y})u(\mathbf{y})\,d\mathbf{y}.$$

The Fourier transform of u^s with respect to x_1 and x_2 yields the coefficient $A(p,q)$. If the evanescent wave contribution $(p^2+q^2>1)$ is neglected in the expression for $A(p,q)$ and only the homogeneous wave contribution $(p^2+q^2<1)$ considered, it is seen that on setting $p=\sin\theta^s\cos\varphi^s$, $q=\sin\theta^s\sin\varphi^s$ that $A(p,q)$ becomes $g(\mathbf{k}^i,\mathbf{k}^s;v)$, where $\theta^i=0$. The scattered directions are restricted to the hemisphere $0\leq\theta^s\leq\pi/2$ Since the coefficient of y_3 namely $(1-p^2-q^2)^{1/2}$ is positive.

MINIMIZATION OF $f(v)$

The inverse problem has now been formulated as a minimization problem, to find the real continuous function on D which minimizes $f(v)$. The Banach space $C_0(D)$ of real continuous functions on D will be employed. Since the assertion that the set $\{v\,|\,v\in C_0(D),\ f(v)\leq f(v_0)\}$, where v_0 is some given function in $C_0(D)$, is bounded, cannot be made, a constraint will be imposed on the problem. Namely, $f(v)$ will be minimized subject to the condition

$$\|v\|\leq\alpha,$$

where $\alpha > 0$ is some given large constant assigned *a priori*. The norm employed here is the usual maximum norm. For future references the following set will be defined

$$S = \{v \mid v \in C_0(D);\ \|v\| \leq \alpha\}.$$

Since S is a closed convex subset of the nonreflexive Banach space $C_0(D)$, the conditional-gradient approach[3,4] will be used to obtain sequences $\{v_n\}$ which minimize $f(v)$ where v_n will be in a dense subset of S, namely a set of equicontinuous functions in S.

With the above approach in mind, the various Gateaux derivatives will be required. Denote the Gateaux derivative of $f(v)$ at v by $f'v$. Hence for $v \in S$ the corresponding linear functional has the value

$$f'v(h) = \lim_{t \to 0} \frac{f(v+th) - f(v)}{t}$$

for every $h \in S$. If the corresponding Gateaux derivative of $g(\mathbf{k}^i, \mathbf{k}^s; v)$ is denoted by $g'v(\mathbf{k}^i, \mathbf{k}^s)$, it then follows

$$f'v = 2\ \mathrm{Re}\left(\sum_{l=1}^{N} W(\mathbf{k}_l^i, \mathbf{k}_l^s)\overline{\Delta g(\mathbf{k}_l^i, \mathbf{k}_l^s)} g'v(\mathbf{k}_l^i, \mathbf{k}_l^s)\right) \tag{9}$$

or

$$f'v = 2\ \mathrm{Re}\left(\int_{K^i \otimes K^s} W(\mathbf{k}^i, \mathbf{k}^s)\overline{\Delta g(\mathbf{k}^i, \mathbf{k}^s)} g'v(\mathbf{k}^i, \mathbf{k}^s) \times d\Omega^i d\Omega^s\right) \tag{10}$$

according to whether $f(v)$ is given by Eq. (7) or Eq. (8), and

$$\Delta g(\mathbf{k}^i, \mathbf{k}^s) = g(\mathbf{k}^i, \mathbf{k}^s; v) - g^e(\mathbf{k}^i, \mathbf{k}^s; v^*). \tag{11}$$

To obtain an explicit expression for $f'v$, note that from Appendix A

$$g(\mathbf{k}^i, \mathbf{k}^s; v_1) - g(\mathbf{k}^i, \mathbf{k}^s; v_2) = \frac{k^2}{4\pi} \int_D (v_1 - v_2)\eta u(\mathbf{k}^i, v_2) u(-\mathbf{k}^s, v_1) d\mathbf{y},$$

where $u(\mathbf{k}, v)$ represents the total field (incident plus scattered) produced by an incident wave in direction $\mathbf{k}$ upon a scatterer whose material properties are given by v. It thus follows that for v and $h \in S$

$$g'v(\mathbf{k}^i, \mathbf{k}^s)(h) = \int_D G(\mathbf{k}^i, \mathbf{k}^s; v) h(\mathbf{y}) d\mathbf{y}, \tag{12}$$

where

$$G(\mathbf{k}^i, \mathbf{k}^s; v) = \frac{k^2}{4\pi} \eta(\mathbf{y}) u(\mathbf{k}^i, v) u(-\mathbf{k}^s, v); \tag{12'}$$

hence $f'v(h)$ has the form

$$f'v(h) = \int_D F(v, \mathbf{y}) h(\mathbf{y}) d\mathbf{y}, \tag{13}$$

where

$$F(v, \mathbf{y}) = 2\,\mathrm{Re}\left(\sum_{l=1}^{N} W(\mathbf{k}_l^i, \mathbf{k}_l^s)\overline{\Delta g(\mathbf{k}_l^i, \mathbf{k}_l^s)} G(\mathbf{k}_l^i, \mathbf{k}_l^s; v)\right) \tag{14a}$$

or

$$F(v, \mathbf{y}) = 2\,\mathrm{Re}\left(\int_{K^i \otimes K^s} W(\mathbf{k}^i, \mathbf{k}^s)\overline{\Delta g(\mathbf{k}^i, \mathbf{k}^s)} G(\mathbf{k}^i, \mathbf{k}^s; v) \times d\Omega^i d\Omega^s\right) \tag{14b}$$

Since the plane wave $\exp(i\mathbf{k}^i \cdot \mathbf{x})$ is an H-differentiable function, and the integral operator in Eq. (4) maps bounded functions into H-differentiable functions, the solution $u(\mathbf{k}^i, x)$ will be an H-differentiable function. Thus it follows that since $\eta(y)$ is H-differentiable, vanishing on the boundary, $G(\mathbf{k}^i, \mathbf{k}^s; v)$, hence $F(v, \mathbf{y})$, will be an H-differentiable function belonging to $C_0(D)$.

In general $f(v)$ is not a convex functional on the set S, hence there will be more than one value of v that gives a local minimum of $f(v)$. A unique value of v yielding an absolute minimum is not to be expected since in general the given set of data is not sufficient to uniquely specify the value of v. One[5] requires the values of $g(k^i, k^s; v^*)$ for all values of $\mathbf{k}^i$ and $\mathbf{k}^s$ $(0 \leq |k| < \infty)$. In addition, errors in the data may obscure the true absolute minimum.

If $\tilde{v}$ is defined as follows

$$\tilde{v} = \min_{h \in S} f'v(h), \tag{15}$$

it is shown[4] that a necessary condition for v to give a minimum is that

$$\tilde{v} = f'v(v). \tag{16}$$

Provided that v is not on the boundary of S, then condition (16) reduces to the familiar condition

$$f'v = 0. \tag{16'}$$

Points v of the set S for which Eq. (16) is satisfied will be called stationary values. These stationary values are generated by the conditional-gradient iteration process described as follows.

Starting from v_1 a uniformly continuous function, a sequence $\{v_n\}$, where $v_n \in S$ is generated in successive steps. In particular, once v_n is obtained, a direction of descent and then amount of descent is chosen to get v_{n+1}. But, to satisfy the constraint, the amount of descent must be restricted to stay within the set S. To be precise, given v_n one finds an $h \in S$ so that

$$\frac{d}{dt} f(v_n + th)\,|_{t=0} = f'v_n(h) = \int_D F(v_n, \mathbf{y}) h(\mathbf{y}) d\mathbf{y}$$

is a minimum. From Eq. (16) it follows that the minimum is given by $\tilde{v}_n$. Since $F(v_n, \mathbf{y}) \in C_0(D)$, it is obvious that $\tilde{v}_n$ is an H-differentiable function in $C_0(D)$ given by

$$\tilde{v}_n = -\frac{F(v_n, \mathbf{y})}{\|F(v_n, \mathbf{y})\|}\,\alpha. \tag{17}$$

Not only has the direction of descent, but also the maximum possible amount has been chosen. The proper amount of descent is now chosen by minimizing the functional

$$P_n(a) = f(v_n + a(\tilde{v}_n - v))$$

for $0 \leq a \leq 1$. Since $f(v)$ is not necessarily convex, the minimum point may be at the end point $a = 1$, or there may be more than one minimum point in which case the smallest value is taken. Let the chosen minimum be a_n; then set

$$v_{n+1} = v_n + a_n(\tilde{v}_n - v_n). \tag{18}$$

It then follows that

$$f(v_{n+1}) < f(v_n);$$

hence $\{v_n\}$ froms a relaxation process.[6]

It is seen that $\{v_n\}$ is a sequence of equicontinuous functions on S; hence it belongs to a bounded conditional compact set and will have a converging subsequence. In order for such a subsequence to converge to a stationary point of $f(v)$, the following Lifschitz condition for the subset of equicontinuous functions in S (see Appendix B) will be used:

$$\|f'v_1 - f'v_2\| \leq L\|v_1 - v_2\|.$$

It follows from the results in Appendix B that the Lifschitz condition, with slight modification of L, can be applied to include the limits of a finite number of converging sequences of equicontinuous functions.

By appropriately modifying the corresponding theorem in Ref. 4 to take into account that although the set S is not weakly compact, the sequences $\{v_n\}$ belong to a bounded conditionally compact set, one has the following:

Theorem: The sequences $\{v_n\}, \{\tilde{v}_n\}$ have the property that

$$\lim_{n\to\infty} f'v_n(v_n - \tilde{v}_n) = 0$$

and the cluster points of $\{v_n\}$ are *stationary* points of $f(v)$ on S.

The above procedure requires the exact determination of a_n. However, this step may be relaxed and the a_n can be chosen to satisfy the following:

$$a_n = \min\left[1,\ \gamma_n \frac{f'v_n(v_n - \tilde{v}_n)}{\|v_n - \tilde{v}_n\|^2}\right] \tag{19}$$

where γ_n satisfies the inequalities

$$\epsilon_1 \leq \gamma_n \leq (2 - \epsilon_2)/L$$

with $0 < \epsilon_1 < 2/L$, $0 < \epsilon_2 < 2 - L\epsilon_1$.

With appropriate modification of proof in Ref. 4, it can be shown that the cluster points of the sequence $\{v_n\}$ with these values of a_n are stationary points.

The above procedure for obtaining stationary points of $f(v)$ involves the direct scattering process For the case where $f(v)$ is given by Eq. (7), one needs to compute $F(v_n, \mathbf{y})$ and the appropriate values of $G(\mathbf{k}_l^i, \mathbf{k}_l^s; v_n)$ for $l = 1, 2, \ldots N$, in order to compute $\tilde{v}_n$ from v_n. But from Eq. (12′) this involves finding the solution of the direct scattering associated with plane waves incident upon a scatterer with $v = v_n$, for a set of incident propagation vectors given not only by $\mathbf{k}_l^i$, but also $-\mathbf{k}_l^s$ for $l = 1, 2, \ldots, N$.

In actual practice one may want to discretize the problem or use approximate direct scattering models. As an example of the latter, one could assume that $v^*(\mathbf{x})$ is a perturbation of some known value $v_0(\mathbf{x}) \in C_0(D)$. In this case one could place a restraint on $(v - v_0)$ so that the appropriate Neumann series of the perturbed integral equation converges. In this case one could work in the real Hilbert space of square integrable functions on D, and have a constraint of the form $k^2\|v - v_0\|_2 \|\mathbb{K}_0\|_2 < 1$, where the norm $\|\ \|_2$ is appropriate norm for the Hilbert space. $\mathbb{K}_0$ is the integral operator associated with the unperturbed equation, the kernel being given by the Green's function. In the next section the linearized version of the perturbation approach is reexamined.

LINEARIZED SYSTEM

The linearized approximation[7] is achieved by treating the unknown quantity $v(\mathbf{x})$ as a small perturbation of a known quantity $v_0(\mathbf{x})$, and retaining only linear terms in the resultant perturbation expansion. In particular, if

$$v(\mathbf{x}) = v_0(\mathbf{x}) + \delta v_1(\mathbf{x}),$$

where δ is a small parameter, when the corresponding expansion for the scattered field

$$u^s(\mathbf{x}) = u_0^s(\mathbf{x}) + \delta u_1^s + O(\delta^2)$$

is substituted into Eq. (2) and coefficients of δ up to the linear terms are equated, one obtains the two equations

$$\Delta u_0^s + k^2[v_0(\mathbf{x}) + 1]u_0^s = -k^2 v_0(\mathbf{x})u^i,$$

$$\Delta u_1^s + k^2[v_0(\mathbf{x}) + 1]u_1^s = -k^2 v_1(\mathbf{x})[u_0^s + u^i].$$

The normal approach is to invert the second equation using the Green's function associated with the operator on the left-hand side of the equation. The resultant expression for the perturbed scattered field appears as a linear functional on $v_1(\mathbf{x})$.

The form of the scattered field for the linearized system can be directly obtained using the Gateaux derivative of $g(\mathbf{k}^i, \mathbf{k}^s; v)$ at v_0. Retaining only the first two terms in the Taylor expansion about v_0, one obtains

$$g(\mathbf{k}^i, \mathbf{k}^s; v_0 + \delta v_1) \sim g(\mathbf{k}^i, \mathbf{k}^s; v_0) + g'v_0(\delta v_1). \tag{20}$$

If the difference between the measured scattered field amplitude and the computed value corresponding to the unperturbed value of v is set equal to $b(\mathbf{k}^i, \mathbf{k}^s)$, i.e.,

$$b(\mathbf{k}^i, \mathbf{k}^s) = g^s(\mathbf{k}^i, \mathbf{k}^s; v^*) - g(\mathbf{k}^i, \mathbf{k}^s; v_0) \tag{21}$$

and δv_1 in Eq. (20) is replaced by $v - v_0$, yielding

$$g(\mathbf{k}^i, \mathbf{k}^s; v) = g(\mathbf{k}^i, \mathbf{k}^s; v_0) + \int_D G(\mathbf{k}^i, \mathbf{k}^s; v_0)(v - v_0)d\mathbf{y},$$

the nonlinear functional $f(v)$ corresponding to Eq. (7) has the following form for the linearized system:

$$f(v) = \sum_{l=1}^{N} W(\mathbf{k}_l^i, \mathbf{k}_l^s) \times \left| \int_D G(\mathbf{k}_l^i, \mathbf{k}_l^s; v_0)(v - v_0)d\mathbf{y} - b(\mathbf{k}_l^i, \mathbf{k}_l^s) \right|^2. \tag{22}$$

A similar result holds for the linear version of Eq. (8), namely

$$f(v) = \int_{K^i \otimes K^s} \int W(\mathbf{k}^i, \mathbf{k}^s) \left| \int_D G(\mathbf{k}^i, \mathbf{k}^s; v_0)(v - v_0)d\mathbf{y} - b(\mathbf{k}^i, \mathbf{k}^s) \right|^2 d\Omega^i d\Omega^s. \tag{23}$$

It can be shown that these expressions for $f(v)$ are convex functions on the set S, i.e., if $v_1, v_2 \in S$ and $v_1 \neq v_2$, then

$$f\left(\frac{v_1 + v_2}{2}\right) \leq \tfrac{1}{2}f(v_1) + \tfrac{1}{2}f(v_2).$$

This fact produces the following result.[4]

Theorem: The sequences $\{v_n\}$ generated by the conditional gradient iteration process for the functional $f(v)$ given by Eq. (22) and (23) has the property

$$\lim_{n\to\infty} f(v_n) = \min_{v\in S} f(v).$$

The stronger result is obtained for the linearized version since $f(v)$ is convex.

Another approach to the linearized version when a finite number of discrete measurements are made, is to note that the nonlinear functional given by Eq. (22) has a minimum when

$$\int_D G(\mathbf{k}_l^i, \mathbf{k}_l^s; v_0)(v - v_0)d\mathbf{y} = b(\mathbf{k}_l^i, \mathbf{k}_l^s), \quad l = 1, 2, \ldots, N.$$

Combined with these N linear functional equations is the constraint

$$\max_{\mathbf{x} \in D} |v(\mathbf{x})| \leq \alpha.$$

The system can be transformed into a system of linear functional equations with positive constraints. Such a system has been treated by Sabatier[8,9] who discretized it by breaking the region D into cubes and hence reduced it to a linear algebraic system which could be solved by the simplex method. It was shown that the maximum "useful" numbers of subdivisions that could be employed was related to the errors in measurements, etc.

BORN APPROXIMATION

An important application of the linearized version occurs when the frequency is sufficiently low or else the scattering medium is sufficiently transparent so that the Born approximation (the retention of the leading term only in the Neumann Series solution) may be used for the direct scattering problem. Here, as pointed out earlier, one can employ the real Hilbert space of square integral functions on D, thus the continuity condition on $v(\mathbf{x})$ may be relaxed, and $v(\mathbf{x})$ is required only to belong to $L^2(D)$. Thus the factor $\eta(\mathbf{y})$ will be suppressed.

Since the Born approximation corresponds to the linearized version with $v_0 \equiv 0$, and

$$g(\mathbf{k}^i, \mathbf{k}^s; v_0) \equiv 0,$$
$$G(\mathbf{k}^i, \mathbf{k}^s; v_0) = \frac{k^2}{4\pi} \exp[i(\mathbf{k}^i - \mathbf{k}^s) \cdot \mathbf{x}],$$

it follows that the linearized versionof the nonlinear function $f(v)$ given by Eq. (23) has the form

$$f(v) = \int_{K^i \otimes K^s} \int W(\mathbf{k}^i, \mathbf{k}^s) |\mathcal{G} v - g^\epsilon(\mathbf{k}^i, \mathbf{k}^s; v^*)|^2 d\Omega^i a\Omega^s, \quad (24)$$

where

$$\mathcal{G} h = \frac{k^2}{4\pi} \int_D \exp[i(\mathbf{k}^i - \mathbf{k}^s) \cdot \mathbf{y}] h(\mathbf{y}) d\mathbf{y}, \quad (25)$$

If the actual material properties of the scatterer is denoted by $v^*(\mathbf{x})$, then the measured scattered far field amplitude in the Born approximation has the form

$$g^\epsilon(\mathbf{k}^i, \mathbf{k}^s; v^*) = \mathcal{G} v^* + \epsilon_1(\mathbf{k}^i, \mathbf{k}^s; v^*), \quad (26)$$

where the error term is a linear combination of errors due to measurements, plus the error in using the Born approximation (the contribution of the remaining terms in the Neumann series).

The special case where the measurements are made at all directions of incidence and scattering will be considered At the same time the weighting factor will be specified as follows:

$$W(\mathbf{k}^i, \mathbf{k}^s) = \frac{1}{\pi^3 2^{3/2}} \quad (|\mathbf{k}^i|^2 - \mathbf{k}^i \cdot \mathbf{k}^s)^{1/2} \quad (27)$$

To simplify analysis, set

$$k(\mathbf{x}, \mathbf{y}) = \left(\frac{k^2}{4\pi}\right)^2 \iint \exp[i(\mathbf{k}^i - \mathbf{k}^s) \cdot (\mathbf{x} - \mathbf{y})] W(\mathbf{k}^i, \mathbf{k}^s) d\Omega^i a\Omega^s, \quad (28)$$

where W is given by Eq. (27) and the integrals are over the unit spheres, and let $\mathcal{T}$ be the linear operator on L prescribed as follows:

$$\mathcal{T} h = \int_D k(\mathbf{x}, \mathbf{y}) h(\mathbf{y}) d\mathbf{y}.$$

If one then sets

$$w(x) = \mathrm{Re} \frac{k^2}{4\pi} \iint \exp[-i(\mathbf{k}^i - \mathbf{k}^s) \cdot \mathbf{x}] g^\epsilon(\mathbf{k}^i, \mathbf{k}^s; v^*) \times W(\mathbf{k}^i, \mathbf{k}^s) a\Omega^i a\Omega^s, \quad (29)$$

it can be shown that expression (24) reduces to

$$f(v) = (v, \mathcal{T} v) - 2(v, w) + f_0, \quad (30)$$

where $f_0 = \int\int W(\mathbf{k}^i, \mathbf{k}^s) |g^\epsilon(\mathbf{k}^i, \mathbf{k}^s; v^*)|^2 d\Omega^i a\Omega^s$ and $(\ ,\ )$ is the inner product associated with the real Hilbert space $L^2(D)$.

For further analysis the properties of the operator $\mathcal{T}$ have to be obtained. In expression (28) change the variables of integration from the spherical angular variables (θ^i, φ^i) and (θ^s, φ^s) to the spherical polar variables (p, θ^p, φ^p) and (q, θ^q, φ^q) by the relation

$$\mathbf{k}^i - \mathbf{k}^s = 2\mathbf{q},$$
$$\mathbf{k}^i + \mathbf{k}^s = 2\mathbf{p},$$

where $\mathbf{q}$, $\mathbf{p}$ are the vectors of length q, p and directions given by (θ^q, φ^q) and (θ^p, φ^p) respectively. It then can be shown that

$$k(\mathbf{x}, \mathbf{y}) = \frac{k^2}{4\pi^4} \int_0^k \int \exp[i2\mathbf{q} \cdot (\mathbf{x} - \mathbf{y})] q^2 a\Omega^q dq,$$
$$= \frac{k^2}{4\pi^4} \iiint \exp[i\,2\mathbf{q} \cdot (\mathbf{x} - \mathbf{y})] H(k - q)\, d\mathbf{q} \quad (31)$$

where $H(x)$ is the Heaviside step function. It is obvious that $k(\mathbf{x}, \mathbf{y})$ is a real symmetric kernel.

Since it follows that

$$(\varphi, \mathcal{T} \varphi) = \frac{k^2}{4\pi^4} \iiint \left| \int_D \exp(i2\mathbf{q} \cdot \mathbf{x}) \varphi(\mathbf{x}) dx \right|^2 \times H(k - q) a\mathbf{q},$$

it is seen that $\mathcal{T}$ is a nonnegative operator. Since $\psi(\mathbf{q}) = \int_D \exp(2i\mathbf{q} \cdot \mathbf{x}) \varphi(\mathbf{x}) a\mathbf{x}$ is an analytic function in each of the components of the vector $\mathbf{q}$, it follows that $\psi(\mathbf{q})$ cannot vanish identically on the ball $|\mathbf{q}| \leq k$ unless $\varphi(\mathbf{x}) = 0$, a.e. Thus it is seen that $\mathcal{T}^{-1}$ exists, but the range space of $\mathcal{T}$ is not closed.

The well-known results of Kantorovich[10] may be used. If $w(\mathbf{x})$ is in the range space of the operator $\mathcal{T}$, then the steepest descent iteration process applied to the functional of Eq. (3) in the real Hilbert space yields a minimizing sequence

$$\lim_{n \to \infty} f(v_n) = f(v^*)$$

where v^* is the solution of

$$\mathcal{T} v^* = w. \quad (32)$$

Note that the results in the previous section using the conditional-gradient method in the Banach space $C_0(D)$ apply to this and will yield the same result. If one works with Eq. (31) directly rather than the functional (30), other iterative processes may be used.[11]

From Eq. (26), (28), and (29) it is seen that

$$w(\mathbf{x}) = \mathcal{J}v^* + w^\epsilon,$$

where w^ϵ is the contribution due to the various sources of errors. Thus if the error term is in the range space of $\mathcal{J}$, i.e., $w^\epsilon = \mathcal{J}\epsilon_v$, then Eq. (32) has the solution

$$v^* = v^* + \epsilon_v$$

and hence one can determine v^* apart from the errors.

It is of interest to compare this result with the theoretical limit that can be obtained by side band holography. It is shown by Wolf[2] that the combined measurements of holography (taking all directions of incidence) yield the quantity $\mathcal{J}v^* H(k - |\xi|)$, where H is the Heaviside step function, and $\mathcal{J}v^*$ is the Fourier transform

$$\mathcal{J}v^* = \int_D \exp(i\boldsymbol{\xi}\cdot\mathbf{x})v^*(\mathbf{x})d\mathbf{x}.$$

From Eq. (31) it is seen that this is just the Fourier transform of $\mathcal{J}v^*$. Here the results derived above indicate that the processing of data will yield better resolution.

COMMENTS

The nonlinear inverse scattering approach considered here has the advantage in that it is capable of utilizing incomplete and diverse scattered data, is stable with regard to errors, and includes many simplified models (e.g., Born approximation) as special cases.

It would be useful to investigate the discretized version of the nonlinear approach given here, as well as the optimum choice of the weighting factors. In addition it would be of interest to extend the analysis to obstacle scattering (as characterized by the Dirichlet or Neumann boundary condition on a closed surface) as well as the corresponding vector problems. In some cases, it may be better to formulate the problem in the time domain as opposed to the frequency domain given here.

APPENDIX A

If $\mathbb{K}$ is the integral operator such that

$$\mathbb{K} = \frac{k^2}{4\pi}\int_D \frac{\exp(ik|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}u(\mathbf{y})d\mathbf{y},$$

then when $v = v_1(\mathbf{x}) \in C_0(D)$, Eq. (14) can be expressed in the form

$$u_1 = u^i + \mathbb{K}\eta v_1 u_1,$$

where $u^i = \exp(i\mathbf{k}^i\cdot\mathbf{x})$ and u_1 is short-hand notation for the solution $u_1 = u(\mathbf{k}^i, v_1)$. It can then be shown that

$$\eta(v_1u_1 - v_2u_2) = \eta v_1\mathbb{K}\eta(v_1u_1 - v_2u_2) + \eta(v_1 - v_2)u_2 \qquad \text{(A1)}$$

Since the operator $\eta v_1\mathbb{K}$ is the complex conjugate of the adjoint operator of $\mathbb{K}\eta v_1$, it follows that Eq. (A1) can be inverted to give

$$\eta(v_1u_1 - v_2u_2) = (I - \eta v_1\mathbb{K})^{-1}\eta(v_1 - v_2)u_2$$

and

$$\begin{aligned}
&\int_D \exp(-i\mathbf{k}^s\cdot\mathbf{x})(v_1u_1 - v_2u_2)\eta d\mathbf{x}\\
&= \int_D \exp(-i\mathbf{k}^s\cdot\mathbf{x})(I - \eta v_1\mathbb{K})^{-1}\eta(v_1 - v_2)u_2 d\mathbf{x}\\
&= \int_D \eta(v_1 - v_2)u_2(I - \mathbb{K}\eta v_1)^{-1}\exp(-i\mathbf{k}^s\cdot\mathbf{x})d\mathbf{x}\\
&= \int_D \eta(v_1 - v_2)u_2 u(-\mathbf{k}^s, v_1)d\mathbf{x}.
\end{aligned}$$

It thus follows that

$$\begin{aligned}
&g(\mathbf{k}^i, \mathbf{k}^s; v_1) - g(\mathbf{k}^i, \mathbf{k}^s; v_2)\\
&= \frac{k^2}{4\pi}\int_D (v_1 - v_2)\eta u(\mathbf{k}^i, v_2)u(-\mathbf{k}^s, v_1)d\mathbf{x}.
\end{aligned}$$

APPENDIX B

Using the notation of Appendix A, it follows from Leis[1] that, for $v \in S$,

$$\|(I - \mathbb{K}\eta v)^{-1}\| \leq C(v).$$

From the relation

$$\begin{aligned}
&\|(I - \mathbb{K}\eta v)^{-1} - (I - \mathbb{K}\eta v_2)^{-1}\|\\
&\leq \frac{\|\mathbb{K}\|C^2(v_1)\|v_1 - v_2\|}{[1 - C(v_1)\|\mathbb{K}\|\,\|v_1 - v_2\|]}
\end{aligned}$$

it follows that $(I - \mathbb{K}\eta v)^{-1}$ is a continuous function of v. Let

$$S' = \{v \mid v \in S;\ v \text{ equicontinuous}\}$$

then S' is a bounded conditionally compact subset of S. It follows that, for $v \in S'$, the inverse operator is uniformly bounded

$$\|(I - \mathbb{K}\eta v)^{-1}\| < M.$$

Hence, for $v \in S'$, one has

$$\|u(\mathbf{k}^i, v)\| < M$$

and from the relation

$$u_1 - u_2 = (I - \mathbb{K}\eta v_1)^{-1}(\mathbb{K}\eta)(v_1 - v_2)u_2$$

that

$$\|u_1 - u_2\| \leq M^2\|\mathbb{K}\|\,\|v_1 - v_2\|.$$

From Eq. (12′) it can be shown that for $v_1, v_2 \in S'$

$$\begin{aligned}
&\|G(\mathbf{k}^i, \mathbf{k}^s, v_1) - G(\mathbf{k}^i, \mathbf{k}^s, v_2)\|\\
&\leq \frac{k^2}{4\pi}\left[\|u(-\mathbf{k}^s, v_1)\|\,\|u(\mathbf{k}^i, v_1) - u(\mathbf{k}^i, v_2)\|\right.\\
&\left. + \|u(\mathbf{k}^i, v_2)\|\,\|u(-\mathbf{k}^s, v_1) - u(-\mathbf{k}^s, v_2)\|\right]\\
&\leq \frac{k^2}{4\pi}M^3\|\mathbb{K}\|\,\|v_1 - v_2\|.
\end{aligned}$$

From expressions (9), (10), and (12) it can be shown that, for v_1, v_2 in the set S', there exists a constant L_1 such that

$$\|F(\mathbf{y}, v_1) - F(\mathbf{y}, v_2)\| \leq L_1\|v_1 - v_2\|,$$

from which follows the Lifschitz condition

$$\|f'v_1 - f'v_2\| \leq L\|v_1 - v_2\|$$

for some appropriate constant L.

Note added in proof: Stronger results can be obtained by adding the term $\lambda\int_D(v - v_0)^2 d\mathbf{x}$ to the nonlinear functional $f(v)$. The conditional-gradient process would then

yield only stationary solutions in a neighborhood of v_0, an initial estimate.

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Completely integrable systems and symplectic actions[a)]

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We study results on a class of completely integrable systems, for instance, with Hamiltonian $H(x,y)=(1/2)\sum_{i=1}^{n} y_i^2+\sum_{i<j}(x_i-y_j)^{-2}+\alpha\sum_{i=1}^{n} x_i^2$, using quotient manifolds induced by symplectic group actions, which enables us to integrate the systems and understand their complete integrability. In addition, we give a natural interpretation for the scattering maps associated with these systems.

1. INTRODUCTION

In this short note we explain the results of "Some finite dimensional integrable systems and their scattering behavior,"[1] by the author, and of Refs. 2–4, in terms of the abstract machinery set up in the paper of Kazhdan, Kostant, and Sternberg, entitled "Hamiltonian group actions and dynamical systems of Calogero type,"[5] which explains systems first discovered by Calogero and Marchioro,[6] and first discussed by Moser,[7].

Briefly, the systems to be discussed have the property that their equations of motion can be expressed as matrix differential equations which can be easily integrated, and moreover, the integration process is seen to occur naturally in a space of much higher dimensionality than the systems in question. The systems to be studied are thus interpreted as quotient systems of the much larger systems, where the quotienting out process is performed by a symplectic action of a group.

The process of quotienting out in mechanics, such as using center of mass coordinates, i.e., ignoring the position of the center mass, is indeed a common practice. We point out that usually quotienting out, or ignoring certain data, is a way of ignoring the symmetries, or integrals of the system, so as to arrive at some basic equations to study. Here the quotienting out does not really involve the integrals, but enables us to pass to the ultimate system to be studied. The integrals are in fact generated in a much more trivial way, for instance through the use of natural Lagrangian submanifolds and simple canonical maps, which of course makes use of the quotient structure. In addition, the so-called scattering maps of these systems have a natural interpretation in this context.

A special case of this symplectic quotienting out process is the coadjoint orbit construction of Kirillov – Kostant (see Ref. 8). This construction is relevant in the n-dimensional Euler spinning top problem of Arnold, as was observed by Dikii in Ref. 9. In addition, the Toda systems and their generalizations, as well as the Korteweg–deVries equation and its generalizations have orbit symplectic structures for their relevant phase spaces. We refer the reader to Kostant,[10] Mumford and Moerbeke,[11] and the author[12] for the former case, and Ref. 12 for the later case.

In the first section we merely summarize the abstract machinery of Ref. 5 of use in the discussion, referring the reader to Ref. 5 and 13, and the paper of Marsden and Weinstein,[8] for a fuller discussion. We then discuss the results of Ref. 1, which entails referring to Ref. 1 frequently. Finally in Sec. 7, we discuss the results of Olshanetsky and Perelomov,[2,3] in the above quotient framework.

2. THE SYMPLECTIC STRUCTURES

We summarize and briefly discuss the necessary abstract machinery needed to discuss Ref. 1. Let (M,ω,G) be a triple, with M an (exact) symplectic manifold with nondegenerate closed 2-form $\omega=d\tau$, and G a Lie group, with elements g, which acts on M with an exact symplectic action. If $\mathcal{L}$ is the Lie algebra of G, with elements denoted by $\mathring{g}$; then the action of G associates with each $\mathring{g}$ the Hamiltonian vector field $\hat{\mathring{g}}$, and the Hamiltonian function $f_{\mathring{g}}(\ )=-\tau(\hat{\mathring{g}})(\ )$, yields a Lie homomorphism, i.e.,

$$\{f_{\mathring{g}_1},f_{\mathring{g}_2}\}=f_{[\mathring{g}_1,\mathring{g}_2]}\quad [\ ,\ ] \text{ the bracket in } \mathcal{L}, \tag{2.1}$$

where $\{\ ,\ \}$ is just the usual Poisson bracket, i.e., if

$$X_f \lrcorner\, \omega = df, \quad \text{then } X_{f_2}(f_1)=\omega(X_{f_1},X_{f_2})=\{f_1,f_2\}. \tag{2.2}$$

We define the moment map of Souriau,

$$\Phi: M\to \mathcal{L}^*, \quad \text{by } \Phi(m)(\mathring{g})=f_{\mathring{g}}(m), \tag{2.3}$$

with $\mathcal{L}^*$ the dual of $\mathcal{L}$. The group G acts on itself by conjugation, hence on $\mathcal{L}$ by the linearization of conjugation, Ad, and on $\mathcal{L}^*$ by $(\mathrm{Ad})^*$; and its easy to see that (2.1) is just the infinitesmal, and hence equivalent version of the relation of equivariance,

$$\Phi\circ g=(\mathrm{Ad}\, g^{-1})^*\circ\Phi. \tag{2.4}$$

We then form the orbit of $\alpha\in\mathcal{L}^*$ under $(\mathrm{Ad})^*$, Θ_α, and assume $V=\Phi^{-1}(\Theta_\alpha)$ is a manifold. It is easy to see V is a coisotropic manifold, i.e., $(TV_x)^\perp\subset(TV_x)$, for all $x\in V$, with $\perp$ denoting perpendicularity with respect to ω, and we can thus form $S=V/[\text{leaves of the foilation induced by } (TV)^\perp]$, taking S to be connected and assuming it to be a manifold. Then as a direct consequence of (2.4), it's not hard to see that S is a covering space of Θ'_α as follows:

$$S\tilde{=}\Theta'_\alpha\times\Theta_\alpha, \quad \Theta'_\alpha=\frac{\Phi^{-1}(\alpha)}{G_\alpha}, \tag{2.5}$$

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where $/G_\alpha$ means we identify elements $x, y \in M$ if they lie on the same G_α orbit, with G_α the isotropy group of α, i.e., the connected subgroup of G which fixes α by its action on M. Incidentally, this shows S is a manifold precisely if Θ'_α is one. By the coisotropy of V, and the transitivity of G on the fibers Θ_α, ω induces a symplectic structure on $\Theta'_\alpha, \omega_\alpha$ (i.e., we shall tacitly assume ω_α is nondegenerate), where $\{\ ,\ \} \to \{\ ,\ \}_\alpha$ is a homomorphism. The structure $(\Theta'_\alpha, \omega_\alpha)$, G shall be our arena of activity.

We note that by (2.1) and (2.2), functions in M which are G invariant induce Hamiltonian flows on M which *pointwise* fix the image of M under Φ, and hence they induce Hamiltonian flows on Θ'_α. In addition, such functions, if they are in involution with respect to $\{\ ,\ \}$ on M, are, via the homomorphism $\omega \to \omega_\alpha$, automatically in involution in Θ'_α, thought of, by their G invariance, as functions on Θ'_α. This ends our discussion of quotient structures.

In preparation, we discuss some M's which shall come up in the examples.

Let F be the linear manifold of $n \times n$ matrices with complex coefficients, and $T^*F = \Phi$ be the cotangent bundle of F, where we shall identify $T^*F \sim F \times F$ via the bilinear $\langle X, Y \rangle = \mathrm{tr}(XY)$. Then the complex symplectic 2-form ω, naturally associated with T^*F is

$$\omega = \sum dX_{ij} \wedge dY_{ji} = \langle dX, dY \rangle,$$

or alternately, we write Hamilton's equations, with Hamiltonian $H = H(X, Y)$, as

$$\dot{X} = H_Y, \quad \dot{Y} = H_X \tag{2.6}$$

where $[H_X]_{ij} = \partial H / \partial X_{ji}$, etc. If we restrict ω to

$$M_1 = T^*\mathcal{L} = \{(X, Y) \mid X = X^*, Y = Y^*\}, \tag{2.7}$$

where * denotes taking the Hermitian adjoint, i.e., $\mathcal{L}$ is just the self-adjoint matrices [which we shall identify with the Lie algebra of the unitary group $G = \mathrm{U}(n, C)$], ω yields a real symplectic structure, with Hamilton's equations remaining as given in (2.6), where it is understood that H is real.

It is interesting to map $\Phi \to \Phi$ via

$$\tau : \begin{vmatrix} X \\ Y \end{vmatrix} \to \begin{vmatrix} X \\ XY \end{vmatrix} = \begin{vmatrix} Z_1 \\ Z_2 \end{vmatrix}, \tag{2.8}$$

and one computes

$$H_X = H_{Z_1} + YH_{Z_2}, \quad H_Y = H_{Z_2} X,$$

$$\dot{Z}_1 = \dot{X} = H_Y, \quad \dot{Z}_2 = (XY)^{\cdot} = H_Y Y - XH_X.$$

Consequently, we may write Hamilton's equations in (Z_1, Z_2) coordinates as

$$\dot{Z}_1 = H_{Z_2} Z_1, \quad \dot{Z}_2 = [H_{Z_2}, Z_2] - Z_1 H_{Z_1}. \tag{2.9}$$

Let us now restrict τ to $T^*\mathrm{U}(n)$, i.e., we identify

$$M_2 = T^*\mathrm{U}(n, C) \tilde{=} \{(Z_1, Z_2) \mid Z_1 Z_1^* = I, Z_2^* = Z_2\}, \tag{2.10}$$

and restrict

$$\tau \to \tau_{|\tau^{-1}(M_2)} = \bar{\tau}.$$

Note $\bar{\tau}$ is invertible, and of course we may just as well identify $\tau^{-1}(M_2)$ with $T^*\mathrm{U}(n)$. In that case, since by the pairing $\langle\ ,\ \rangle$, X, Y are the usual dual coordinates of $T^*\mathrm{U}(n)$, (2.9) restricted to M_2 precisely yields Hamilton's equations for the natural symplectic structure of $T^*\mathrm{U}(n)$. We must however put in the factor i due to our identification of the Lie algebra of $\mathrm{U}(n)$ with self-adjoint matrices, or equivalently we may think of time as being purely imaginary in (2.9). We omit the necessary, but easy verification that (2.9) restricted to M_2 automatically perserves M_2, which is sufficient to insure the restricted ω is symplectic.

3. EQUATIONS OF MOTION FOR THE SIMPLEST SYSTEM

We now apply the discussion of Sec. 2. We shall let (M, ω, G) of Sec. 2 be $(M_1, (dX, dY), \mathrm{U}(n))$ of Sec. 2. Since $M_1 = T^*\mathcal{L} \sim \mathcal{L} \times \mathcal{L}$, $\mathcal{L}$ the Lie algebra of $\mathrm{U}(n)$, $\mathrm{U}(n)$ acts naturally on $\mathcal{L}$ via Ad, i.e., by conjugation, which extends to a Hamiltonian action on $T^*\mathcal{L}$:

$$U : (X, Y) \to (UXU^{-1}, UYU^{-1}), \quad U \in \mathrm{U}(n),$$

of which the linear version is

$$\dot{U} : (X, Y) \to ([\mathring{U}, X], [\mathring{U}, Y]) \in TM_{1(X,Y)}.$$

Hence, by (2.3), and the above

$$\Phi(X, Y)(\mathring{U}) = f_{\mathring{U}}(X, Y) = \langle [\mathring{U}, X], Y \rangle = \langle [X, Y], \dot{U} \rangle,$$

and so by the identification of $\mathcal{L}$ with $\mathcal{L}^*$ through $\langle\ ,\ \rangle$

$$\Delta_\alpha \equiv \Phi^{-1}(\alpha) = \{(X, Y) \mid [X, Y] = \alpha\}, \tag{3.1}$$

and we shall once and for all pick α such that

$$[\alpha]_{jk} = i(1 - \delta_{jk}), \quad \text{i.e.,} \quad \alpha = i\{v^* \otimes v\},$$

with $v \in R^n$, $v = (1, 1, 1 \ldots, 1)^T$. Note that the isotropy subgroup $G_\alpha = \{U \mid U \propto U^{-1} = \alpha\}$, and we shall define the effective reduced subgroup

$$G_0 = \{U \mid U(v) = v\}, \text{ with Lie algebra } \mathcal{L}_0 = \{B \mid B(v) = 0\}. \tag{3.2}$$

In Ref. 5 it is shown by a simple linear algebra argument that if $[X, Y] = \alpha$, we can always find a unique $U \in G_0$ such that

$$UXU^{-1} = \mathrm{diag}(x_1, x_2, \ldots, x_n) \equiv \bar{x}, \quad x_i < x_{i+1}, \text{ all } i,$$

$$[UYU^{-1}]_{jk} = \delta_{jk} y_j + i(1 - \delta_{jk})(x_j - x_k)^{-1} \equiv \bar{y} \tag{3.3}$$

and hence $\Theta'_\alpha = \Phi^{-1}(\alpha)/G_\alpha$ is effectively coordinatized by $((x_1, x_2, \ldots, x_n), (y_1, \ldots, y_n)) = (x, y)$; and moreover it is shown in Ref. 5, by a local argument, that

$$\omega \to \omega_\alpha = \sum_{i=1}^{n} dx_i \wedge dy_i, \quad \text{i.e.,} \quad (x, y) \tag{3.4}$$

form a set of canonical coordinates. Hence in this case, Θ'_α, and thus S is a manifold (see Sec. 2), and ω_α is nondegenerate, and hence symplectic.

We now wish to find functions on Θ'_α, and by the discussion in Sec. 2, functions of the form

$$H = H(X, Y) = \mathrm{tr}[P(X, Y)], \tag{3.5}$$

with $P(\cdot, \circ)$ a noncommuting polynomial in its arguments, will certainly do. If we take (3.5) as a Hamiltonian function on M_1, then (2.6) yields for Hamilton's equa-

tions,

$$\dot{X}=h_1(X,Y),\quad \dot{Y}=h_2(X,Y) \tag{3.6}$$

with $h_i(\cdot,\cdot)$, $i=1,2$, polynomials in their arguments, uniquely determined by $P(\cdot,\cdot)$. As mentioned, $H=\mathrm{tr}[P(X,Y)]$ automatically can be thought of as a function on Θ'_α, in fact via

$$h(x,y)=\mathrm{tr}[P(\bar{x},\bar{y})]; \tag{3.7}$$

and we wish to determine the analog of (3.6) for the system on Θ'_α with Hamiltonian (3.7), or to put it another way, we shall determine how (3.6) transforms in Θ'_α.

So assume we are given initial data for Hamiltonian's equation with Hamiltonian $h(x,y)$ in Θ'_α, which corresponds to $(\bar{x}(0),\bar{y}(0))$, which we may identify, and thus set equal to, $(X(0),Y(0))$ in M_1. Under the Hamiltonian $h(x,y)$, $(\bar{x}(0),\bar{y}(0))\to(\bar{x}(t),\bar{y}(t))$, and correspondingly under the Hamiltonian $H(X,Y)$, $(X(0),Y(0))\to(X(t),Y(t))$. By the previous remarks, we must have

$$X(t)=U\bar{x}(t)U^{-1},\quad Y(t)=U\bar{y}(t)U^{-1},\quad U=U(t), \tag{3.8}$$

with $U(t)\in G_0$ [see (3.2)] uniquely defined, as the $H(X,Y)$ flow in the big manifold M_1 descends to the $h(x,y)$ flow in the little manifold Θ'_α through quotienting out via G_0. Define $B(t)\in\mathcal{L}_0$ [see (3.2)] by $\dot{U}=-UB$, and so by (3.6) and (3.8),

$$\dot{X}=U\delta\bar{x}U^{-1}=h_1(X,Y)=Uh_1(\bar{x},\bar{y})U^{-1},$$

where $\delta\bar{x}=\dot{\bar{x}}-[B,\bar{x}]$; and so we have

$$\delta\bar{x}=h_1(\bar{x},\bar{y}),\quad \delta\bar{y}=h_2(\bar{x},\bar{y}). \tag{3.9}$$

As a consequence of Hamiltonian's equations on Θ'_α, $\dot{x}=(\partial/\partial x)[h(x,y)]$, $\dot{y}=-(\partial/\partial y)[h(x,y)]$, and thus we see how (3.6) is transformed in Θ'_α. Note that from the definitions of δ, (3.9), and $B(v)=0$ [see (3.2)], we can immediately compute the unexpected functional dependence, $B(t)=B(\bar{x}(t),\bar{y}(t))$, since $\bar{x}$ is a diagonal matrix.

We specialize to the case $H=H_f=\mathrm{tr}[f(Y)]$, for which we compute [see (3.6)] $h_1(X,Y)=f'(Y)$, $h_2=0$, and thus conclude from (3.6) and (3.9),

$$\dot{X}=f'(Y),\quad Y'=0, \tag{3.10}$$

$$\delta\bar{x}=f'(\bar{y}),\quad \delta\bar{y}=0. \tag{3.11}$$

Since (3.10) is immediately solvable, we have in fact solved (3.11) by the use of (3.8).

We also note that since the H_f's clearly are in involution on M_1, being function only of Y, that by the homomorphism $\omega\to\omega_\alpha$, the h_f's, $h_f=\mathrm{tr}[f(\bar{y})]$, are in involution on Θ'_α, and in fact are generated by n independent functions $h^{(j)}=\mathrm{tr}[(\bar{y})^j]$, $j=1,2,\ldots,n$. Thus $h=\mathrm{tr}(\frac{1}{2}y^2)$ gives rise to a completely integrable Hamiltonian system.

4. SCATTERING MAPS

Upon inspection, one observes that the map

$$\eta:(X,Y)\to(Y,X),\quad \eta|_{\Delta_\alpha}:\Delta_\alpha\to\Delta_{-\alpha},\quad \text{[see (3.1)]}, \tag{4.1}$$

is a canonical map with multiplier -1 in M_1, and hence so is its projection η_p in Θ'_α, since $\omega\to\omega_\alpha$ is a homomorphism. This map, η_p, is precisely the scattering map for system (3.11), with $f(s)=\frac{1}{2}s^2$, which is discussed in Ref. 1, Theorem 6, as was observed by J. Moser (in a personal communication). More precisely, in the above case, (3.11) with $f(s)=\frac{1}{2}s^2$, one shows the time evolution of the system is given by

$$(x,y)=(qt+p+O(t^{-1}),p+O(t^{-2})),\quad t\to+\infty,$$

with

$$\eta_p:(x(0),y(0))\to(q,p).$$

Similarly one defines the $\pi/4$ rotation map

$$\hat{\eta}:(X,Y)\to 2^{-1/2}(X+Y,X-Y),\quad \hat{\eta}|_{\Delta_\alpha}:\Delta_\alpha\to\Delta_{-\alpha}, \tag{4.2}$$

which is easily seen to be canonical with multiplier -1 on M_1 (here one uses that X,Y are Hermitian), and the corresponding canonical projection, $\hat{\eta}_p$ on Θ'_α. If $h(x,y)=\frac{1}{2}\mathrm{tr}(\bar{y}^2-\bar{x}^2)$ in (3.7), then the time evolution of the system (3.9) is given by

$$(x(t),y(t))=2^{-1/2}\times(q^+e^{+t}+p^+e^{+t},q^+e^{+t}-pe^{+t})+O(e^{-2|t|}),$$

$$t\to\pm\infty$$

with

$$\hat{\eta}_p(x(0),y(0))=(q,p).$$

This is shown in Ref. 1, Theorem 4. Moreover, as one easily checks

$$\eta=\hat{\eta}\circ\rho\circ\hat{\eta}^{-1},\quad \rho:(X,Y)=(X,-Y),$$

hence

$$\hat{\eta}_p=\hat{\eta}_p\circ\rho_p\circ\hat{\eta}_p^{-1},$$

and by (3.3), $\rho_p(x,y)=(x,-y)$.

Note that we have shown, by the time reversibility of system (3.9), that $\eta_p:(q^-,p^-)\to(q^+,p^+)$. These latter statements are shown in Ref. 1, Theorems 5 and 6.

5. TWO EQUIVALENT SYSTEMS

We now investigate the systems on Θ'_α with Hamiltonians respectively

$$h_1(x,y)=\mathrm{tr}[f(\bar{x}\cdot\bar{y})], \tag{5.1a}$$

$$h_2(x,y)=\mathrm{tr}\{f(\tfrac{1}{2}[\bar{x}+\bar{y}]\cdot[\bar{x}-\bar{y}])\}. \tag{5.1b}$$

By the canonical map $\hat{\eta}_p$ of Sec. 4, it is only necessary to investigate case (a), and then via $\hat{\eta}_p$, transpose the results to case (b). Also, via the transformation formalism (3.8), and (3.6)↦(3.9), it is only necessary to study the equations on the full manifold M_1, rather than the quotient manifold Θ'_α. The formalism says substitute δ for d/dt, and $(\bar{x},\bar{y})$ for X,Y), which enables one to compute the generator B, and solve the equation on the big manifold, M_1, and via (3.8), to pass to the solution on the quotient manifold Θ'_α.

We thus need only study the system on M_1 with Hamiltonian

$$H_1=H_f(X,Y)=\mathrm{tr}[f(XY)], \tag{5.2}$$

and we first show the H_f's are in involution. Specifically, assume

$$H^{(1)}=\mathrm{tr}[f_1(XY)],\quad H^{(2)}=\mathrm{tr}[f_2(XY)],$$

then, taking increments,

$$\delta H^{(1)}=\mathrm{tr}\{f_1'(XY)\cdot[\delta X\cdot Y+X\cdot\delta Y]\}+O^{(2)},$$

where $O^{(2)}$ means terms of at least second order; and we have

$$H_X^{(1)} = Y \cdot f_1'(XY), \quad H_Y^{(1)} = f_1'(XY) \cdot X, \tag{5.3}$$

etc., for $H^{(2)}$. By (2.6) and (2.2), the Poisson bracket $\{\ ,\ \}$ of $H^{(1)}, H^{(2)}$ is given by [where $\langle A, B\rangle = \mathrm{tr}(AB)$] $\{H^{(1)}, H^{(2)}\} = \langle H_X^{(1)}, H_Y^{(2)}\rangle - \langle H_Y^{(1)}, H_X^{(2)}\rangle$, and thus substituting in (5.3), we find

$$\{H^{(1)}, H^{(2)}\} = \langle Yf_1', f_2'X\rangle - \langle f_1'X, Yf_2'\rangle$$
$$= \mathrm{tr}(f_1'f_2'XY) - \mathrm{tr}(f_1'f_2'XY) = 0,$$

where we have used $[f_2'(XY), XY] = 0$, and so $\{H^{(1)}, H^{(2)}\} = 0$.

We have thus, through $\hat{\eta}$, shown the H_2's, $H_2 = H_f = \mathrm{tr}\{f(\frac{1}{2}[X+Y]\cdot[X-Y]\}$, are in involution, and thus by the homomorphism $\omega \to \omega_\alpha$, so are the $\{\mathrm{tr}[f(\overline{xy})]\}$'s $\{\mathrm{tr}[f(\frac{1}{2}[\bar{x}+\bar{y}]\cdot[\bar{x}-\bar{y}])]\}$'s, respectively; and so $\mathrm{tr}(\frac{1}{2}\bar{x}\bar{y}^{-})$, $\mathrm{tr}(\frac{1}{2}[\bar{x}+\bar{y}]\cdot[\bar{x}-\bar{y}])$, respectively give rise to completely integrable Hamiltonian systems on Θ_α', as was observed proven in Ref. 1. This is, thus, the second and more pleasant proof of that fact.

Now by (2.6) and (5.3), Hamiltonian's equations of the system of (5.2) are

$$\dot{X} = f'(XY)\cdot X, \quad \dot{Y} = -Yf'(XY) \tag{5.4}$$

and since $(XY)^{\cdot} = 0$ as a consequence of $[f'(XY), XY] = 0$, we immediately integrate (5.4) to obtain

$$X = \exp(f'(X_0Y_0)t)\cdot X_0, \quad Y = Y_0 \cdot \exp(-f'(X_0Y_0)t), \tag{5.5}$$

where the subscript o denotes evaluation at $t = 0$. Thus by (3.9), the corresponding equations on Θ_α' for the systems of (5.1a) are

$$\delta\bar{x} = f'(\overline{xy})\cdot\bar{x}, \quad \delta\bar{y} = -\bar{y}f'(\overline{xy}), \tag{5.6}$$

while (3.8) implies the time evolution of (5.6) is given by

$$\mathrm{diag}(x_1, x_2, \ldots, x_n)(t) = U^{-1}\exp(f'(X_0Y_0)t)\cdot X_0U, \text{ etc.} \tag{5.7}$$

The canonical map $\hat{\eta}$ (5.4), implies the corresponding equations and time evolution for the system with Hamiltonian $H_2 = \mathrm{tr}[f(\frac{1}{2}[X+Y]\cdot[X-Y])]$ are

$$(X+Y)^{\cdot} = -f'(\tfrac{1}{2}[X+Y]\cdot[X-Y])\cdot[X+Y],$$
$$(X-Y)^{\cdot} = [X-Y]\cdot f'(\tfrac{1}{2}[X+Y]\cdot[X-Y]),$$

with

$$\{\tfrac{1}{2}[X+Y]\cdot[X-Y]\}^{\cdot} = 0, \tag{5.8a}$$

and

$$(X+Y) = [\exp -\{tf'(\tfrac{1}{2}[X_0+Y_0]\cdot[X_0-Y_0])\}]\cdot[X_0+Y_0],$$
$$(X-Y) = [X_0-Y_0]\cdot[\exp\{\tfrac{1}{2}tf'[X_0+Y_0]\cdot[X_0-Y_0]\}], \tag{5.8b}$$

where the changing of signs $t \to -t$, comes about because $\hat{\eta}$ is the canonical multiplier -1. We now use (3.8) and (3.9) to transpose (5.8) to Θ_α', i.e., system (5.1b), in particular concluding

$$2\delta\bar{x} = [\bar{x}, f'] - [f', \bar{y}]_+, \quad 2\delta\bar{y} = [\bar{y}, f'] - [f', \bar{x}]_+, \tag{5.9}$$

where $[A, B]_+ = AB + BA$, $f' = f'(\frac{1}{2}[\bar{x}+\bar{y}]\cdot[\bar{x}-\bar{y}])$. Note the simplicity of (5.8) and (5.9), when $f(s) = s$. We could equally well study the systems gotten by "stretching" $X \to \mu\cdot X$, in (5.1) and (5.2), which tend to have compact behavior and thus give rise to periodic solutions for μ purely imaginary, see Ref. 1, in fact for $f(s) = s$, $\mu = \sqrt{-1}$, all solutions are periodic with one and the same nonprimitive period.

Note that our studying the case $H = \mathrm{tr}[f(XY)]$, $h = \mathrm{tr}[f(\overline{xy})]$, makes it unnecessary to study the (Sutherland) case where our manifold is

$$T^*U(n, C) \tilde{=} \{(U, R) \mid UU^* = I,\ R = R^*\},$$

and our Hamiltonian is $H(U, R) = H_f = \mathrm{tr}[f(R)]$, with Hamilton's equations given by (2.9), $(U, R) = (Z_1, Z_2)$; for after the change $t \to it$, we would get the same formal results as (5.4)–(5.7), including the involution statement, via the map τ, (2.8), where we identify $(X, XY) = (Z_1, Z_2)$ with (U, R). We note that the condition $(X, Y) \in \Delta_\alpha$, namely $[X, Y] = \alpha$ is transformed into $[U, U^{-1}R] = \alpha$, i.e., $R - U^{-1}RU = \alpha$.

6. YET ANOTHER SYSTEM ON θ_α'

We now discuss the system of Sec. 6 of Ref. 1.

One may either regard the Hamiltonian of this system on Θ_α' as

$$h_1 = \mathrm{tr}[\tfrac{1}{2}(\overline{xy})^2 + \bar{x}], \tag{6.1}$$

or

$$h_2 = \mathrm{tr}(\tfrac{1}{2}\bar{x}\bar{y}^2\bar{x} + \bar{x}), \tag{6.2}$$

as h_1, h_2 differ by a constant. Of course in the full manifold the corresponding Hamiltonians,

$$H_1 = h[\tfrac{1}{2}(XY)^2 + X], \tag{6.3}$$

$$H_2 = \mathrm{tr}[\tfrac{1}{2}(XY^2X) + X], \tag{6.4}$$

are far from identical. Although it is shown in Ref. 1 that (6.1) and (6.2) are completely integrable systems, we shall not show that (6.3) and (6.4) are completely integrable systems, in fact we have not been able to do this.

We shall study both (6.3) and (6.4) and then relate them in case the associated differential equations on Θ_α' have the same initial data. Since the calculations are so similar to those of Sec. 5, we just give the results. For simplicity we set $XY = Z$. Then with the Hamiltonian of (6.3) we calculate, from (2.6),

$$\dot{X} = ZX, \quad \dot{Z} = -X,$$

and since $[X, Y] = \alpha$, $(YX)^{\cdot} = -X$, we have $\frac{1}{2}(XY^2X) + X = e_1$, e_1 a constant, and thus we arrive at, again using $[X, Y] = \alpha$,

$$\tfrac{1}{2}Z^2 - \tfrac{1}{2}Z\alpha - \dot{Z} = e_1. \tag{6.5}$$

Letting $Z = -2a_1^{-1}\dot{a}_1$, we find $\ddot{a}_1 = \frac{1}{2}a_1e_1 - \frac{1}{2}\dot{a}_1\alpha$, hence we have

$$\begin{pmatrix} a_1 \\ \dot{a}_1 \end{pmatrix} = \begin{pmatrix} a_1(0) \\ \dot{a}_1(0) \end{pmatrix} \cdot \exp C_1 t, \tag{6.6}$$

$$C_1 = D_1(X, Y) = \begin{bmatrix} 0, & I \\ \frac{1}{4}(XY^2X) + \frac{1}{2}X, & -\alpha/2 \end{bmatrix} \text{ at } t = 0. \tag{6.7}$$

For the Hamiltonian of (6.4), we find

$$\dot{Z} - [\tfrac{1}{2}YX, Z] = -X, \quad \dot{X} - [\tfrac{1}{2}YX, X] = \tfrac{1}{2}(XZ + ZX),$$

which motivates us to define the derivation δ,

$$\delta(\cdot)=\frac{d}{dt}(\cdot)-[\tfrac{1}{2}YX,\cdot],$$

and thus we have from the above,

$$\delta Z=-X,\quad \delta X=\tfrac{1}{2}(XZ+ZX). \tag{6.8}$$

Clearly, if $U(0)=I$, $\dot U=-U(\frac{1}{2}YX)$, we have the following rule of transformations for matrices $A=A(t)$: If $\hat A\equiv UAU^{-1}$, then $(d/dt)^j\hat A=U\delta^j AU^{-1}$. From (6.8) we conclude, using that δ is a derivation,

$$\delta(\tfrac{1}{2}Z^2+X)=0,\quad \delta(\tfrac{1}{2}Z^2-\delta Z)=0; \tag{6.9}$$

hence by our rule of transformation,

$$\tfrac{1}{2}\hat Z^2-\dot{\hat Z}=e_2,\quad e_2 \text{ a constant};$$

and thus letting $\hat Z=-2a_2^{-1}\dot a_2$, we find

$$\dddot a_2=\tfrac{1}{2}a_2e_2,$$

i.e.,

$$\begin{pmatrix}a_2\\ \dot a_2\end{pmatrix}=\begin{pmatrix}a_2(0)\\ \dot a_2(0)\end{pmatrix}\cdot\exp C_2t,$$

$$C_2=D_2(X,Y)=\begin{bmatrix}0, & I\\ \tfrac{1}{4}(XY)^2+\tfrac{1}{2}X, & 0\end{bmatrix}\ \text{at } t=0. \tag{6.10}$$

We now consider the case where the $X(0)$ of both systems are the same in Θ'_α, and moreover $x_1(0)>0$. Then since both Eqs. (6.3) and (6.4) are the same as seen in Θ'_α, they both must have the same long term behavior of X as is projected down into Θ'_α. In Ref. 1, Sec. 6, it is shown that system (6.3) and (6.4) have the following long term "scattering" behavior,

$$(\log x,xy)=(\pm\lambda t+\beta^\pm+O(t^{-1}),\pm\lambda+O(t^{-2})),\quad t\to\pm\infty,$$

where $\log x=(\log x_1,\dots,\log x_n)$, $xy=(x_1y_1,\dots,x_ny_n)$. By arguments in that same section, it's clear that the spectrum of C_1, or alternately C_2, precisely carry the data λ, and hence we must have

$$D_1(X,Y)\sim D_2(X,Y),$$

where $\sim$ denotes spectral equivalence. By (6.7), (6.10), and (3.8), this implies

$$D_1(\bar x\,\bar y)\sim D_2(\bar x,\bar y). \tag{6.11}$$

Moreover it follows from (6.5) and (6.9) that $D_1(X,Y)$, $D_2(X,Y)$ are isospectral matrices of the differential equations (6.3 and (6.4) respectively, and so in particular $D_1(\bar x,\bar y)$, $D_2(\bar x,\bar y)$ are for the (6.1) and (6.2) flow; and thus we arrive at

$$D_1(\bar x(0),\bar y(0))\sim\lim_{t\to\pm\infty}D_1(\bar x(t),\bar y(t))\sim\lim_{t\to\pm\infty}D_2(\bar x(t),\bar y(t)). \tag{6.12}$$

This yields the scattering behavior of system (6.1) and (6.2) as discussed in Corollaries 11.2, 11.3, of Ref. 1, which essentially maintains that the system scatters as if it is completely decoupled, and is just constrained to maintain a fixed order on the line.

7. THE GENERALIZATIONS OF OLSHANETSKY AND PERELOMOV

We now apply the considerations of Sec. 2, and Ref. 5, to generalizations of the Calogero–Moser systems in the context of complex semisimple Lie algebras as considered by Olshanetsky and Perelomov.[2,3] We shall recover their results along the way. They actually work in the setting of real Lie algebras, but the natural setting for a full analysis is the complex Lie algebras and their real conpact decompositions. We remark that we shall make seemingly stronger hypotheses than they do. As this section is in effect an abstraction of the work of the previous sections, we shall tend to sketch arguments in order to avoid unnecessary redundancy. We first need to enumerate some well-known facts about Lie algebras which we mention without proof (see Ref. 14).

Let $\tilde{\mathcal{L}}$ be a semisimple Lie algebra over C, the complex numbers, with connected Lie group $\tilde G$ and with (nondegenerate) Killing form $\langle X,Y\rangle=\mathrm{tr}(\mathrm{ad}X\,\mathrm{ad}Y)$. Note $\langle\cdot,\cdot\rangle$ has the following important properties (where $[\cdot,\cdot]$ denotes the Lie bracket):

$$\langle X,[Y,Z]\rangle=\langle Y[Z,X]\rangle=\langle Z,[X,Y]\rangle, \tag{7.1}$$
$$\langle \mathrm{Ad}_gX,\mathrm{Ad}_gY\rangle=\langle X,Y\rangle,\ g\in\tilde G.$$

Let h be a Cartan subalgebra of $\tilde{\mathcal{L}}$, with $\tilde\Delta$ the corresponding set of nonzero roots, and Δ the subset of roots which are positive with respect to some ordering. Pick root vectors $E_\beta\subset\tilde{\mathcal{L}}^\beta$, $\tilde{\mathcal{L}}^\beta$ a root subspace corresponding to the root $\beta\in h^*$, having the following properties:

$$[E_\beta,E_{-\beta}]=H^{(\beta)}\in h,\quad \langle H^{(\beta)},H^{(\beta)}\rangle=1,$$
$$[H,E_\beta]=(\beta\langle H\rangle)\cdot E_\beta\equiv H_\beta\cdot E_\beta,\quad \text{for all } H\in h. \tag{7.2}$$

Let $\mathcal{L}\subset\tilde{\mathcal{L}}$ denote the compact R-*linear* subspace

$$\mathcal{L}=\sum_{\beta\in\Delta}R\cdot(iH^{(\beta)})+\sum_{\beta\in\Delta}R\cdot(E_\beta-E_{-\beta})+\sum_{\beta\in\Delta}R\cdot(i(E_\beta+E_{-\beta})); \tag{7.3}$$

and thus we have the R-*linear* direct sum

$$\tilde{\mathcal{L}}=\mathcal{L}+(i\mathcal{L}),\ \text{and moreover } [\mathcal{L},\mathcal{L}]\subset\mathcal{L}. \tag{7.4}$$

Let G denote the connected Lie group with Lie algebra $\mathcal{L}$.

From (7.2), we have $\langle\cdot,\cdot\rangle_{|\mathcal{L}\times\mathcal{L}}\to R$ and by the nondegeneracy of $\langle\cdot,\cdot\rangle,\langle\cdot,\cdot\rangle$ restricted to $\mathcal{L}\times\mathcal{L}$, $(i\mathcal{L})\times(i\mathcal{L})$, respectively, is nondegenerate (and real). This allows us to identify $T^*(i\mathcal{L})\cong(i\mathcal{L})\times(i\mathcal{L})\equiv M_3$. From (7.4), G acts on $(i\mathcal{L})$ via the adjoint action, which one extends symplectically to $T^*(i\mathcal{L})$. Hence for the triple (M,ω,G), of Sec. 2 we take $((i\mathcal{L})\times(i\mathcal{L}),\ d\langle X,dY\rangle,G)$, where we take (X,Y) as running coordinates on $M_3=(i\mathcal{L})\times(i\mathcal{L})$. As in Sec. 3 we compute the associated moment map, using (7.1), $\Phi(X,Y)(\dot g)=\langle[X,Y],\dot g\rangle$; hence by the nondegeneracy of $\langle\cdot,\cdot\rangle_{|\mathcal{L}\times\mathcal{L}}$ $\Phi^{-1}(\alpha)=\{(X,Y)\,|\,[X,Y]=\alpha\}$, $\alpha\in\mathcal{L}$.

We now pick a very special α, $\alpha=\sum_{\beta\in\Delta}c_\beta(E_\beta-E_{-\beta})$, $c_\beta\neq0$, real, $\beta\in\Delta$, satisfying:

Property A: Let G_α be the connected isotropy group of α with Lie algebra $\mathcal{L}_\alpha$, which we assume is specified by a relation of the form

$$\mathcal{L}_\alpha=\{\dot g\,|\,P_h\dot g+L(I-P_h)\dot g=0,\ \dot g\in\mathcal{L}_\alpha\},$$

where $P_h:\tilde{\mathcal{L}}\to\tilde{\mathcal{L}}$ is specified by $P_h(\Sigma f_\beta H_\beta+\Sigma l_\beta E_\beta)=\Sigma f_\beta H_\beta$ [see (7.3) and (7.4)] I is the identity operator in $\tilde{\mathcal{L}}$, and L is some linear map; moreover, if $[X,Y]=\alpha$, then

there exists $g \in G_0$ such that $\mathrm{Ad}_g X \equiv \bar{x} \in h$ (which shall imply $\bar{x}$ is regular). The only freedom in the element g is that we may specify which Weyl chamber $\bar{x}$ is contained in, and we shall always take it to be the positive Weyl chamber with respect to the ordering, h^+; and then only a finite number of choices remain for g.

Using Property A of α, we can easily compute $\Theta'_\alpha = \Phi^{-1}(\alpha)/G_\alpha$. For if $[X, Y] = \alpha$, we pick $g \in G_0$ such that $\mathrm{Ad}_g X = \bar{x}$, hence $\mathrm{Ad}_g Y = \tilde{y} + \Sigma_{\beta \in \Delta} c_\beta \bar{x}_\beta^{-1}(E_\beta + E_{-\beta}) \equiv \bar{y}$, $\tilde{y} \in h$. Note automatically $\beta(\bar{x}) = \bar{x}_\beta \neq 0$, $\beta \in \Delta$, hence $\bar{x}$ is regular. We shall specify g uniquely by requiring $\bar{x}_\beta > 0$, $\beta \in \Delta$. We now pick an orthonormal basis of h, with respect to $\langle \cdot, \cdot \rangle$, $\{H_1, H_2, \ldots H_n\}$, and define $\bar{x} = \Sigma_{i=1}^n x_i H_i$, $\tilde{y} = \Sigma_{i=1}^n y_i H_i$. From the previous remarks it follows that we may take $(x_1, \ldots, x_n, y_1, \ldots, y_n) = (x, y)$ as coordinates on Θ'_α, noting that they are constrained by the open relations $\bar{x}_\beta > 0$, $\beta \in \Delta$, to lie in the positive Weyl chamber.

We claim that the symplectic structure induced on Θ'_α is $\omega \to \omega_\alpha = \Sigma_{i=1}^n dx_i \wedge dy_i$. For if $P_h X = \Sigma X_i H_i$, $P_h Y = \Sigma Y_i H_i$, $\omega = \langle dX, dY \rangle = \Sigma dX_i \wedge dY_i + \{(I - T \in X,\ (I - P_h) Y \text{ terms}\}$; hence if we show for $X_\epsilon = \bar{x} + \epsilon T$, $T \in (1 - P_h)(i\mathcal{L})$, that $[X_\epsilon, Y_\epsilon] = \alpha$ implies $\mathrm{Ad}_{g_\epsilon} X_\epsilon = \bar{x} + \Theta(\epsilon^2) \in h^+$, $g_0 = e$, $g \in G_0$, we will have proven our (local) assertion up to "second order," which is sufficient (see the argument given in Ref. 5). First by the regularity of $\bar{x}$ (and implicitly the uniqueness of g_ϵ), it is easy to see— in fact by sharpening the argument to be given— that g_ϵ is smooth in ϵ. Let $g_\epsilon = e + \epsilon V + \Theta(\epsilon^2)$, with the notation having the obvious meaning. As we must have $\mathrm{Ad}_{g_\epsilon}(\bar{x} + \epsilon T) = \bar{x} + \epsilon \bar{x}_1 + \Theta(\epsilon^2) \in h$, for all ϵ small, it follows, upon expanding the left side of the equation in ϵ, that $[V, \bar{x}] + T = \bar{x}_1 \in h$; but $\bar{x} \in h$ implies $[V, \bar{x}] \in (1 - P_h)\mathcal{L}$, hence $P_h([V, \bar{x}] + T) = 0$. Thus $\bar{x}_1 = 0$, as was to be shown.

For Hamiltonians on M_3 which induce Hamiltonians on Θ'_α, we pick the G invariant functions $H = H(X, Y) = \mathrm{tr}[P(\mathrm{ad}X, \mathrm{ad}Y)]$, with P a noncommuting polynomial of its arguments. As is usual, we define the gradient of $H \in C^1(M_3)$ as follows: $\delta H \equiv \langle \delta X, H_X \rangle + \langle H_Y, \delta Y \rangle$, H_X, $H_Y \in (i\mathcal{L})$. This uniquely specifies H_X, H_Y. Note the adjoint invariance of H, hence of δH [and the adjoint invariance of $\langle \cdot, \cdot \rangle$ in (7.1)], implies

$$\mathrm{Ad}_g H_X(X, Y) = H_X(\mathrm{Ad}_g X, \mathrm{Ad}_g Y), \tag{7.5}$$

similarly for H_Y. In particular if $H = (a/2)\langle X, X \rangle + (b/2) \times \langle Y, Y \rangle$, $H_X = aX$, $H_Y = bY$. By the form of $\omega = \langle dX, dY \rangle$, Hamilton's equation on M_3 for the Hamiltonian H are

$$\dot{X} = H_Y(X, Y), \quad \dot{Y} = -H_X(X, Y); \tag{7.6}$$

which upon using $\mathrm{Ad}_g \bar{x} = X$, $\mathrm{Ad}_g \bar{y} = Y$ and (7.5), are easily seen, as in Sec. 3, to transform on Θ'_α to the equations

$$\delta \bar{x} = H_Y(\bar{x}, \bar{y}), \quad \delta \bar{y} = -H_X(\bar{x}, \bar{y}), \tag{7.7}$$

with

$$\delta(\cdot) = \frac{d\cdot}{dt} - [B, \cdot], \quad \dot{g} \equiv -(L_g)_* B(t), \quad g(0) = e,$$

where $L_g : g_1 \mapsto g g_1$. Of course we have as usual on Θ'_α,

$$\frac{dx_i}{dt} = \frac{\partial h(x, y)}{dy_i}, \quad \frac{dy_i}{dt} = -\frac{\partial h}{\partial x_i}, \quad i = 1, \ldots n,$$

$$h = h(x, y) = H(\bar{x}, \bar{y}).$$

Since $\bar{x} \in h$ is regular, (7.7) implies $[B, \bar{x}] = (1 - P_h) H_Y(\bar{x}, \bar{y})$; and thus determines $(1 - P_h)B$, and hence B, since $B \in \mathcal{L}_\alpha$, as a function of t through $B = B(x, y)$.

Since automatically the $H^{(j)} = (1/2j)\mathrm{tr}(\mathrm{ad}\bar{y})^{2j}$, $j = 1, \ldots, n$, are in involution on M_3, so are the $h^{(j)} = (1/2j)\mathrm{tr}(\mathrm{ad}\bar{y})^{2j}$, $j = 1, \ldots, n$, on Θ'_α; and hence they give rise to a completely integral system on Θ'_α. The corresponding Hamiltonian differential equations are (where the subscript 0 shall denote initial conditions), $\dot{X} = H_Y^{(j)}(Y)$, $\dot{Y} = 0$, hence $X(t) = H_Y^{(j)}(Y_0) \cdot t + X_0$, $Y(t) = Y_0$ on M_3. Therefore, on Θ'_α we have $\delta \bar{x} = H_Y^j(\bar{y})$, $\delta \bar{y} = 0$, hence $\bar{x}(t) = \mathrm{Ad}_{g^{-1}(t)}([H_Y^{(j)}(\bar{y}_0)]t + \bar{x}_0)$, $\bar{y}(t) = \mathrm{Ad}_{g^{-1}} \bar{y}_0$, $\delta \cdot = (d \cdot / dt) - [B_j, \cdot]$, for an appropriate $g(t)$. In particular for $j = 1$, $H_Y^{(1)}(Y) = Y$, and thus the above implies

$$\delta \bar{x} = \bar{y}, \quad \delta \bar{y} = 0, \quad \text{hence } \delta(\bar{x} - t\bar{y}) = 0; \tag{7.8}$$

which in particular implies $(1 - P_h)B_1 = \Sigma_{\beta \in \Delta} \bar{x}_\beta^{-2} c_\beta \times (E_\beta - E_{-\beta})$. It is easy to show (see Ref. 1), that

$$(x(t), y(t)) \mapsto (qt + p + \Theta(t^{-1}), p + \Theta(t^{-2})), \quad t \to \infty; \tag{7.9}$$

and that as a consequence of (7.8) and (7.9) the canonical map $(x, y) \mapsto (q, p)$ is just the projection of the canonical map $\eta : (X, Y) \mapsto (Y, X)$ onto Θ'_α (se Sec. 4 of Ref. 1). Note that from (7.2) $h^{(1)} = \frac{1}{2}\langle \bar{y}, \bar{y} \rangle = \frac{1}{2}\Sigma_{i=1}^n y_i^2 + \Sigma_{\beta \in \Delta} c_\beta^2 \bar{x}_\beta^{-2}$, which is just the Calogero–Moser potential of Olshanetsky and Perelomov. We remark that the proof of *complete* integrability given here is the only algebraic proof we know of, i.e., the only one that doesn't depend on the scattering map.

If we let $H = \frac{1}{2}(\langle Y, Y \rangle - a^2 \langle X, X \rangle)$, then Hamilton's equations on M_3 are $\dot{X} = Y$, $\dot{Y} = a^2 X$; which transform to the equations $\delta \bar{x} = \bar{y}$, $\delta \bar{y} = a^2 \bar{x}$, on Θ'_α, with the appropriate $\delta(\cdot) = (d \cdot / dt) - [B, \cdot]$. Since $\delta \bar{x} = \bar{y}$, $B = B(x, y) = B_1(x, y)$, the B_1 going with the Hamiltonian $h^{(1)}$. Note the Hamiltonian function on Θ'_α is $h^{(1)} - (a^2/2)\Sigma_{i=1}^n x_i^2$. Since on M_3, $2X(t) = (X_0 + a^{-1}Y_0)e^{ta} + (X_0 - a^{-1}Y_0)e^{-ta}$, $2\bar{x}(t) = \mathrm{Ad}_{g^{-1}}[(\bar{x}_0 + a^{-1}\bar{y}_0)e^{ta} + (\bar{x}_0 - a^{-1}\bar{y}_0)e^{-ta}]$, $\dot{g} = -(L_g)_* B$, etc., for $\bar{y}(t)$.

The scattering maps for this system are discussed precisely as in Sec. 4 using the maps η and $\hat{\eta}$, the crucial tool being $\delta[(\bar{y} \pm a\bar{x})e^{\mp at}] = 0$, (see Ref. 1). The preceding equation also implies $\mathrm{tr}[\mathrm{ad}(\bar{y} + a\bar{x}) \cdot \mathrm{ad}(\bar{y} - a\bar{x})]^v$, $v = 1, \ldots, n$, are integrals for the above system. If we let $a = ib$, b real, in the above equations, we get a periodic system with period $2\pi/b$.

We now consider the Sutherland type systems. Namely, let us identify, with the usual symplectic structure, $T^*G \cong G \times (i\mathcal{L}) \equiv M_4$, via the (nondegenerate) inner product $-i\langle \cdot, \cdot \rangle_{|(i\mathcal{L}) \times (i\mathcal{L})}$, where M_4 has the running coordinates (Q, R). The group G acts on itself by conjugation which extends naturally to a symplectic action on $T^*G = M_4$, via $g : (Q, R) \mapsto (gQg^{-1}, \mathrm{ad}_{g^{-1}} R)$; and thus we have for the triple of Sec. 2, $(M, \omega, G) = (G \times (i\mathcal{L}), d(i\langle R, Q^{-1}dQ \rangle), G)$ (see Ref. 2). Note that the linearized version of this group action about (e, R) is just the previous group action. The discussion we give here is towards a different purpose than the one in Sec. 2, and of necessity proceeds differently, although the formulas are of course related. Since $i\omega_{|(Q,R)} = -\langle dR, Q^{-1}dQ \rangle + \langle R, Q^{-1}dQ \wedge Q^{-1}dQ \rangle$, if (η_1, β_1), (η_2, β_2) are elements of $T(T^*G)_{|(Q,R)} \cong \mathcal{L} + (i\mathcal{L}) = \mathcal{L}$, we have

$$i\omega((\eta_1, \beta_1), (\eta_2, \beta_2))_{|(Q,R)} = \langle R, [\eta_1, \eta_2] \rangle + (\langle \beta_2, \eta_1 \rangle - \langle \beta_1, \eta_2 \rangle). \tag{7.10}$$

Given $H=H(Q,R)\in C^1(M_4)$, we define the gradient of H in the ususal way (which is slightly different from the way of Sec. 2),

$$i\delta H=\langle \delta R, H_R\rangle+\langle H_Q, Q^{-1}\delta Q\rangle,\quad H_R\in \mathcal{L},\quad H_Q\in(i\mathcal{L}); \tag{7.11}$$

and from the definition $\omega(X_H, Y)\equiv Y(H)$, one finds

$$X_H=(L_Q)_*H_R\partial_Q+([R,H_R]-H_Q)\partial_R; \tag{7.12}$$

and thus we have the Poisson bracket $\{\cdot,\cdot\}$,

$$\begin{aligned}\{F^{(1)},F^{(2)}\}&=\omega(X_{F^{(1)}},X_{F^{(1)}})=i\langle R,[F_R^{(2)},F_R^{(1)}]\rangle\\&\quad+i(\langle F_Q^{(1)},F_R^{(2)}\rangle-\langle F_Q^{(2)},F_R^{(1)}\rangle).\end{aligned} \tag{7.13}$$

Note that if $H=H(R)$ is an adjoint invariant function, then if $g(t)=e+\dot{g}t+\Theta(t^2)$, $0=(d/dt)(iH(\mathrm{Ad}_gR))=\langle[\dot{g},R],H_R\rangle=\langle R,[H_R,\dot{g}]\rangle$, for all $\dot{g}\in\mathcal{L}$, hence by (7.13) all adjoint invariant functions of R are in involution.

As is easily computed (see Ref. 5), the moment map for our action is given by $\Phi(Q,R)=\mathrm{Ad}_QR-R$ [note $\Phi(Q,R)\in(i\mathcal{L})$. We now pick an $\alpha=\sum_{\beta\in\Delta}ic_\beta(E_\beta-E_{-\beta})$, $c_\beta\neq0$, real, $\beta\in\Delta$, satisfying:

Property B: Let $\mathcal{L}_\alpha$ be specified by a relation of the form given in Property A, such that if $\mathrm{Ad}_QR-R=\alpha$, then there exists a $g\in G_0$ such that $gQg^{-1}\equiv\exp(2i\bar{q})$, $\bar{q}\in h$ (which shall imply $\bar{q}$ is regular). The only freedom in g is that we may specify which Weyl chamber $\bar{q}$ is contained in, and we shall always take it to be in the positive Weyl chamber, h^+, with respect to the ordering, and then only a finite number of choices remain for g.

As usual we compute $\Theta'_\alpha=\Phi^{-1}(\alpha)/G_\alpha$. If $\mathrm{Ad}_QR-R=\alpha$, by Property B there is a $g\in G_0$, such that $gQg^{-1}\equiv\exp\equiv\exp2i\bar{q}$, $\bar{q}\in h$. If we apply Ad_g to the equation $\mathrm{Ad}_QR-R=\alpha$, we have $\mathrm{Ad}_{(gQg^{-1})}(\mathrm{Ad}_gR)-(\mathrm{Ad}_gR)=\alpha$; and so upon making use of the identity $\mathrm{Ad}_{\exp H}E_\alpha=e^{H\alpha}\cdot E_\alpha$, $H\in h$, which is a consequence of (7.2), we conclude,

$$\mathrm{Ad}_qR=\bar{p}+\sum_{\beta\in\Delta}ic_\beta\frac{(e^{-i\bar{q}_\beta}E_\beta+e^{i\bar{q}_\beta}E_{-\beta})}{(e^{i\bar{q}_\beta}-e^{-i\bar{q}_\beta})}\equiv\bar{r},\quad\bar{p}\in h.$$

Note that automatically $\bar{q}_\beta\neq n\pi$, $n\in Z$, $\beta\in\Delta$, and thus in particular $\bar{q}$ is regular; and by property B, we may also assume $\bar{q}_\beta>0$, $\beta\in\Delta$. If now $\{H_1,\dots,H_n\}$ is an orthonormal basis of h, let $\bar{q}=\sum_{i=1}^n q_iH_i$, $p=\sum_{i=1}^n\bar{p}_iH_i$, then from the previous remarks we may take $(q_1,\dots,q_n,p_1,\dots,p_n)=(q,p)$ as coordinates on Θ'_α, subject to the open relations $\bar{q}_\beta>0$, $\bar{q}_\beta\neq n\pi$, $n\in Z$, $\beta\in\Delta$.

The symplectic structure $\omega\to\omega_\alpha=2\sum_i^n dq_i\wedge dp_i$. To establish this (local) fact, it is sufficient to show that at the point $(Q_\epsilon,R_\epsilon)=(\exp(2i\bar{q}+\epsilon T),R_\epsilon)$, $\bar{q}\in h$, $P_hT=0$, $\Phi(Q_\epsilon,R_\epsilon)=\alpha$, the $\langle R,[\eta_1,\eta_2]\rangle$ piece in (7.10) is really "second order" in ϵ. This reduces to showing, as in the previous case, that for the (unique) $g_\epsilon=e+\epsilon V+\Theta(\epsilon^2)$ discussed in Property B, $g_\epsilon\exp(2i\bar{q}+\epsilon T)g_\epsilon^{-1}=\exp[2i\bar{q}+\Theta(\epsilon^2)]$, which upon linearizing about $\epsilon=0$ is just the familiar fact that $P_h([V,2i\bar{q}]+T)=0$.

We now consider the adjoint invariant Hamiltonians on M_4, $H^{(j)}=(1/2j)\mathrm{tr}(\mathrm{ad}R)^{2j}$, $j=1,2,\dots,n$, which as discussed before, are in involution. Since the $H^{(j)}$'s are G invariant functions, they project down to Hamiltonians, $h^{(j)}(q,p)=(1/2j)\mathrm{tr}[(\mathrm{ad}\bar{r})^{2j}]$, $j=1,\dots,n$, on Θ'_α; which moreover are in involution, thus giving rise to a completely integrable system. From (7.12), the $H^{(j)}$'s lead to the Hamiltonian differential equations on M_4, $\dot{R}=0$, $\dot{Q}=(L_Q)_*H_R$ (where we have used the fact $[R,H_R^{(j)}]=0$); which has the solution $R(t)=R_0$, $Q(t)=(L_{Q_0})_*\exp((H_R(R_0)t)$. To study the equations projected to Θ'_α, set $g^{-1}Qg(t)=\exp[2i\bar{q}(t)]$, $g(0)=e$, $\dot{g}\equiv-(Lg)_*B_j$. The previous equations imply, in a now familiar manner, $\bar{r}=\mathrm{Ad}_{g^{-1}}\bar{r}_0$, $q=-(i/2)\exp^{-1}(g^{-1}(L_{Q_0}\exp[H_R(r_0)t)]g)$, $Q_0=\exp(2i\bar{q}_0)$. The associated differential equtions for $\bar{r}$, $\bar{q}$, are easily computed using $g^{-1}\dot{Q}g=\exp(2i\bar{q})$, $\mathrm{Ad}_{g^{-1}}R=\bar{r}$, and the adjoint invariance of $H=H^{(j)}(R)$, i.e., $\mathrm{Ad}_gH_R^{(j)}(R)=H_R^{(j)}(\mathrm{Ad}_gR)$. They are found to be

$$\dot{\delta\bar{r}}=0,\quad 2i\dot{\bar{q}}=\mathrm{ad}_QB_j-B_j+H_R(\bar{r}_0),\quad Q=\exp(-2i\bar{q}). \tag{7.14}$$

In the case of $j=1$, $H^{(1)}(R)=iR$, and (7.14) implies $(1-P_h)B_1=-\frac{1}{4}\sum_{\beta\in\Delta}c_\beta(E_\beta-E_{-\beta})\sin^{-2}\bar{q}_\beta$, which thus determines B_1. We also note that $\dot{\alpha}=0$, $\delta\dot{\alpha}=0$, hence $\delta(r+\frac{1}{2}\alpha)=0$ for all the above differential equations; and so $r^*=r+\frac{1}{2}\alpha=p+\frac{1}{2}\sum_{\beta\in\Delta}c_\beta\cot q_\beta(E_\beta+E_{-\beta})$ satisfies the "Lax equation" $\delta r^*=0$ for all the above flows. Finally note that $h^{(1)}=\frac{1}{2}\langle\bar{r},\bar{r}\rangle=\frac{1}{2}\sum p_i^2+\frac{1}{4}\sum_{\beta\in\Delta}c_\beta^2\cot^2\bar{q}_\beta$, the "Sutherland" potential. We may of course scale these algebraic equations, $q\to aq$, and take a purely imaginary to get the noncompact case, or let $a\to0$ to get the x^{-2} potential, which corresponds to linearizing the group action about (e,R).

We remark that although Properties A and B imply the computational "Lax" criteria of Olshanetsky and Perelomov, (see Refs. 2, 3), and hence seem stronger, we suspect that in fact they are equivalent. In practice, from the remarks in Ref. 5, it is clear that in order to find α satisfying Properties A and B, one should look for α's whose orbits have dimension $2\{\mathrm{rank}_{\mathcal{C}}\mathcal{L}\}$ under the adjoint action of G. Thus one would expect that the α's in Properties A and B are the same up to the factor $\sqrt{-1}$. It is of course an interesting question to investigate Θ'_α's for symplectic actions other than the ones discussed here, and hopefully find more integrable systems. Finally, we mention that given a concrete matrix representation of $\tilde{G}$, we can of course represent the preceding equations as matrix equations; and hence recover results of preceding sections.

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Formal quark binding and geometric strings

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Geometric quantization is applied to a line bundle over spacetime with structure group $GL(2,\mathbb{C})/SL(2,\mathbb{C})$ and curvature form determined by the Ricci tensor. The Ricci form is interpreted as the Hamiltonian form for a particle moving on a string associated with a harmonic oscillator spectrum. Strings are characterized as minimal surfaces, and quarks as the gradients of minimal immersions of surfaces in a three-dimensional spatial hypersurface, leading to a model of a baryon as the intersection of three such surfaces, and their associated quarks.

I. INTRODUCTION

In a previous paper[1] it was suggested that the Ricci form of a line bundle appearing in geometric quantization could be used explicitly as the Hamiltonian form of some formal mechanical system, and that in the special case of general relativity with $T_{\mu\nu}$ having a U(3) generalized duality symmetry group[2] this could be relevant to the theory of quark binding. The purpose of this article is to investigate this question in more detail.

The geometric quantization[3] is based on the methods of Segal[4] and Kostant.[5,6] The former approach uses the metric tensor, $g_{\mu\nu}$, of space—time, together with the complex structure J implicit in the definition of two-component spinors, to define local creation and annihilation operators for vectors and spinors. The choice of complex structure J defines a reduction of the bundle of general linear frames, with structure group $GL(4,\mathbb{R})$, to that of complex linear frames, with group $GL(2,\mathbb{C})$, whilst the further reduction to the bundle of spin frames (up to a sign) with group $SL(2,\mathbb{C})$ is determined by a section of a line bundle, $L(M)$, with structure group $GL(2,\mathbb{C})/SL(2,\mathbb{C})$. Line bundles can be classified by the integral cohomology class of their Ricci curvature form, and this form is used in the Kostant approach for quantizing real scalar functions, in this case on space—time. The Segal type of approach is equivalent to this if the Kähler form $g(X,JY)$ is cohomologically equivalent to the Ricci form $R(X,JY)$ for all vector fields X, Y on space—time. The difference between the two forms is given by the tracefree Ricci tensor $U_{\mu\nu} \equiv R_{\mu\nu} - \frac{1}{4}Rg_{\mu\nu}$, again contracted with J, and it is this object which forms the basis of the Petrov—Plebanski classification of second rank symmetric tensors in terms of their eigenvalues.[2,7]

The phase space of the formal mechanical system is the four-dimensional tangent space to space—time, and the configuration space a two-dimensional subspace related to the polarization in Kostant quantization. The interpretation of the system is considered in Sec. II of this paper using Hamiltonian functions and Kostant quantization, showing that these functions are associated with formal harmonic oscillators. This, together with the two-dimensional configuration space, is suggestive of strings in dual resonance theory,[8] and in Sec. III this correspondence is investigated. The usual string Lagrangian leads to the characterization of the surfaces of evolution of strings as minimal surfaces, and in this paper an alternative definition, as the vanishing of the mean curvature vector, is used in conjunction with analyticity arguments with respect to J to show how such surfaces arise in geometric quantization. This approach is used to describe a formal point particle with energy—momentum tensor of Plebanski type $[T-3S]_{(2)}$ in terms of quark representations of an SU(3) group, and formal strings.

Finally, Sec. IV compares the spinning string formalism of geometric quantization with elementary aspects of supergauge theory, but in this paper no attempt is made to deal with problems of string theory associated with normal ordering or ghost elimination.

II. HAMILTONIAN FUNCTIONS

In elementary classical mechanics the Hamiltonian form of a single particle moving in $R^n \times R^1$ can be expressed as

$$\Omega_0 = \sum_{i=1}^{n} dp_i \wedge dq^i - dh \wedge dt, \tag{2.1}$$

where (p_i, q^i) are momentum and position coordinates, and the Hamiltonian, h, for this motion is related to a Lagrangian L by

$$h = L - \sum_{i=1}^{n} \frac{\partial L}{\partial \dot{q}^i}\ \dot{q}^i, \tag{2.2}$$

$$p_i = \frac{\partial L}{\partial \dot{q}^i}. \tag{2.3}$$

In general any nondegenerate closed 2-form Ω can be interpreted as a Hamiltonian form, and as the Ricci form is closed by virtue of the Bianchi identities it may be considered in this role in regions of space—time where it does not vanish; if degeneracy occurs, then the mechanical system still exists, but is subject to constraints.

The classification of Ricci forms is based on the Plebanski classification[3] of the corresponding Ricci tensor, whereby the type of the tensor is denoted $[\lambda_0 - \lambda_1 - \lambda_2 - \lambda_3]_{(n)}$, where λ_a, $0 \leq a \leq 3$, are the eigenvalues and (n) the degree of the minimal polynomial of the corresponding matrix. Four generic types exist: $[T\text{-}S_1\text{-}S_2\text{-}S_3]_{(4)}$, $[Z\text{-}\bar{Z}\text{-}S_1\text{-}S_2]_{(4)}$, $[2N\text{-}S_1\text{-}S_2]_{(4)}$, and $[3N\text{-}S]_{(4)}$ together with degenerate subtypes, where Z denotes a complex eigenvalue, T a real eigenvalue

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whose eigenspace contains a timelike eigenvector, N an eigenvalue with a null, but no timelike eigenvectors, and S an eigenvalue with only spatial eigenvectors. In this paper only the first of these generic types, and that, for a Riemannian space would be the only type, is considered. In terms of eigenvectors, V^a, $0 \leq a \leq 3$, the Ricci form Ω for this type can be written

$$\Omega = (T - S_3)dV^0 \wedge dV^3 - (S_1 + S_2)\, dV^1 \wedge dV^2, \tag{2.4}$$

where the two bivectors are preserved up to an orientation by J. Comparing this with (2.1) shows that Ω formally describes a particle moving in the V^2 direction with Hamiltonian $(T\text{-}S_3)V_3$ and momentum $-(S_1 + S_2)V_1$, so that energy and momentum are both linearly proportional to displacements, but in different directions. The other Plebanski types differ from (2.4) by all containing terms of the general nature $dp \wedge dt$ and $dh \wedge dq$ which vitiate this simple interpretation.

Further investigation of the mechanical properties of the system requires consideration of Hamiltonian functions for symmetries of Ω, and their Kostant quantization. A vector field X generates a symmetry of Ω if the corresponding Lie derivative $\pounds_X$ vanishes

$$\pounds_X \Omega = 0. \tag{2.5}$$

The Lie derivative can be expressed in terms of exterior derivation, d, and contraction with respect to X, $X \rfloor$, by

$$\pounds_X \Omega = X \rfloor d\Omega + d(X \rfloor \Omega). \tag{2.6}$$

Since Ω is closed, symmetries must satisfy

$$d(X \rfloor \Omega) = 0 \tag{2.7}$$

and this leads to the exact sequence on which the Kostant quantization is based

$$0 \to \mathbb{C} \to \mathbb{C}^\infty(M) \xrightarrow{\delta} A(M) \xrightarrow{i} A_0(M) \xrightarrow{j} \mathrm{U}(M), \tag{2.8}$$

where $\mathbb{C}^\infty(M), A(M), A_0(M)$, and $\mathrm{U}(M)$ denote, respectively, smooth complex functions, globally Hamiltonain vector fields, locally Hamiltonian vector fields, and complex vector fields, all on space–time M. $A_0(M)$ consists of vector fields X, which satisfy (2.7) and $A(M)$ those X for which $X \rfloor \Omega$ is exact

$$A(M) = \{X \in A_0(M) \,|\, (X \rfloor \Omega) = d\varphi\}, \quad \varphi \in C^\infty(M). \tag{2.9}$$

The maps i and j are inclusions, and δ is the prequantization map

$$\delta : \varphi \to X_\varphi, \tag{2.10}$$

where X_φ is defined by (2.9).

Symmetries of the Ricci tensor generated by homogeneous vector fields have been classified by Plebanski using generalized duality invariances of the tracefree tensor $U_{\mu\nu}$ which can be represented as subgroups of orthonormal transformations SO(3, 3) of $\mathbb{R}^6$ curvature bivector space. For $U_{\mu\nu} \neq 0$, the maximal group is U(3) for type $[T\text{-}3S]_{(2)}$, which preserves a complex structure on $\mathbb{R}^6$, and consists of SO(3, $\mathbb{R}$) vierbein rotations of the spatial eigenvectors, their duals in $\mathbb{R}^6$ and the pure duality transformations which are diagonal elements of U(3), of which the latter do not generate symmetries of the trace except for phase rotations generated by J corresponding to hermiticity of $R_{\mu\nu}$. For $[T\text{-}S_1\text{-}S_2\text{-}S_3]_{(4)}$, J invariance is the only symmetry, whilst for types with degenerate eigenvalues rotations in the planes of equal pairs of eigenvectors are symmetries. Any vector field X can be expanded locally[9] in terms of the nonholonomic basis $\{V^a\}$, $0 \leq a \leq 3$

$$X = \sum_{a=0}^{3} \eta^a \frac{\partial}{\partial V^a} \tag{2.11}$$

$$\eta^a \approx \sum_{k=0}^{\infty} \frac{1}{k!} \sum_{a_1,\ldots,a_k=0}^{3} \eta^a_{a_1 \cdots a_k} V^{a_1} \cdots V^{a_k}. \tag{2.12}$$

The vector field X generates an automorphism of an integrable kth order G structure iff for each fixed set $(a_2 \cdots a_k)$ the element $\eta^a_{a_1 \cdots a_k}$ belongs to the Lie algebra of G. For a vector field X generating rotations only the $k = 1$ terms in (2.12) are nonzero, leading to the usual description of rotations by

$$\left(V^a \frac{\partial}{\partial V^b} - V^b \frac{\partial}{\partial V^a}\right)$$

etc., but for the J invariance in four dimensions the full group is the second-order group U(2, 2) with first-order part GL(2, $\mathbb{C}$), whilst in the atypical case of two dimensions[10] there is an infinite parameter group important in string theory (see Sec. IV). J-phase transformations are purely first order and generated by

$$\sum_{i=1}^{2} \left(z^i \frac{\partial}{\partial z^i} - \bar{z}^i \frac{\partial}{\partial \bar{z}^i}\right),$$

where

$$z^1 = \frac{1}{\sqrt{2}}(V^0 + V^3), \quad z^2 = \frac{1}{\sqrt{2}}(V^1 + iV^2) \tag{2.13}$$

and the second-order elements of U(2, 2,) are special conformal transformations which give symmetries of $U_{\mu\nu}$ but not of $R_{\mu\nu}$.

From this the Hamiltonian functions for members of $A(M)$ can be written down by inspection using (2.4) and (2.9). For $[T - S_1 - S_2 - S_3]_{(4)}$ there is only one Hamiltonian function, φ_J, where

$$\varphi_J = \tfrac{1}{2}\{(T - S_3)z^1\bar{z}_1 - (S_1 + S_2)z^2\bar{z}_2\} \tag{2.14}$$

which in the special case of an Einstein space, where the tracefree combinations of eigenvalues are zero, reduces to

$$\varphi_J = \tfrac{1}{4}R(z^1\bar{z}_1 + z^2\bar{z}_2). \tag{2.15}$$

For $[2T - 2S]_{(2)}$, which describes a general electromagnetic field if the trace is zero, (2.14) becomes

$$\varphi_J = \tfrac{1}{4}Rz^1\bar{z}_1 - Sz^2\bar{z}_2 \tag{2.16}$$

and there is also a Hamiltonian function, φ_{12}, for rotation in the (1 – 2) plane

$$\varphi_{12} = S\{(V^1)^2 - (V^2)^2\} \tag{2.17}$$

and in the $R = 0$ electromagnetic case, Ω is only of second rank with φ_J and φ_{12} becoming equivalent. In the case of $[T - 3S]_{(2)}$ there are two Hamiltonian functions, φ_J and φ_{12} given by (2.14) with equal S_i, $0 \leq i \leq 3$, and (2.17). The (1 – 3) and (2 – 3) rotations have the effect of changing J, and it was suggested previously[1] that in this case space–time admits three complex structures differing by SO(3, $\mathbb{R}$) transformations: Such a structure is known as a quaternionic structure[11,12] and requires the

vanishing of the Ricci curvature. If the Ricci curvature is nonzero an almost quaternionic structure can still occur, but in this case only one of the three linearly independent complex structures can be integrable, and hence usable in the Kostant quantization.

Each of the Hamiltonian functions above is formally similar to that of a harmonic oscillator, and the Kostant quantization of such a system has already been considered in the literature.[6] In order to overcome problems associated with curvature and lack of square integrability, the prequantization map δ is replaced by a quantization map $\tilde{\delta}$, where δ acts on sections s of the line bundle $L(M)$ by covariant derivation

$$\delta_\varphi s = (\nabla_{X_\varphi} - 2\pi i\varphi)s \tag{2.18}$$

and $\tilde{\delta}_\varphi$ is given by

$$\tilde{\delta}_\varphi = \delta_\varphi + \mathcal{L}_{X_\varphi} v_x^{1/2} \tag{2.19}$$

where v denotes the volume element on a polarization $F_x(M)$ of the tangent space $T_x(M)$ at $x \in M$, where $F_x(M)$ is chosen to give an irreducible representation, and the Hilbert space of square integrable functions W, where

$$W = \{\psi \in \Gamma(L \otimes L^F) \mid \nabla_X \varphi = 0 \forall X \in F_x(M)\}, \tag{2.20}$$

where $\Gamma(L \otimes L^F)$ denotes the space of sections of the line bundle defined locally by the product of fibres of $L(M)$ with the volume elements $(v_x)^{1/2}$ over $x \in M$. Solving the eigenvalue equation for the operator $\tilde{\delta}_\varphi$, where φ is the Hamiltonian function, φ_J or φ_{12} leads to a harmonic oscillator spectrum, with a zero point energy coming from the volume element term in $\tilde{\delta}_\varphi$. For (2.14) the eigenvalues e_J satisfy for the special case of an Einstein manifold

$$e_J = (2\pi)^{-1}(N+1), \quad N \text{ an integer} \tag{2.21}$$

corresponding to a two-dimensional oscillator, whilst in the general case the two vibrations are nondegenerate, and φ_J has a one-dimensional spectrum. Because of the rotational nature of the Hamiltonian vector fields their eigenvalues have an angular momentum interpretation suggesting a Regge-trajectory like relation, and to this end a string interpretation is considered in the next section.

III. MINIMAL SURFACES

A special case arising in the theory of polarizations over space– time is that in which the distributions $\{F_x\}$, $x \in M$, are surface forming, and furthermore form a minimal surface. For real vector fields X, $Y \in \{F_x\}$, the condition that they are locally surface forming is according to Frobenius theorem that they are involutive, i.e.,

$$[X, Y] \in F_x(M) \quad \forall X, Y \in F_x(M) \tag{3.1}$$

which is satisfied by any real polarization F, leaving only the minimal condition to be considered. For complex vector fields (3.1) is not sufficient, but as any complex submanifold of a Kähler manifold is necessarily minimal[13] we consider minimal surfaces directly in what follows.

The physical significance of minimal surfaces comes from the observation of Nambu[14] that a vibrating string is the simplest model giving the harmonic oscillator spectrum of the factorizable Veneziano amplitude in dual resonance theory

$$\alpha' M^2 = \sum_n n\, a^\dagger_{\mu n} a^\mu_n, \tag{3.2}$$

where α' is the slope of the Regge trajectory, M the invariant mass, and n the occupation number of the Fock space with creation and annihilation operators $a, a^\dagger$. The string motion can be described by either of two actions I_1 and I_2

$$I_1 = \frac{1}{4\pi\alpha'}\int_0^\tau d\sigma \left[\left(\frac{\partial x^\mu(\sigma,\tau)}{\partial\tau}\right)^2 - \left(\frac{\partial x^\mu(\sigma,\tau)}{\partial\sigma}\right)^2\right], \tag{3.3}$$

$$I_2 = \frac{1}{2\pi\alpha'}\int_{\tau_1}^{\tau_2} d\tau \int_0^\tau d\sigma \left[\left(\frac{\partial x^\mu}{\partial\tau}\,\frac{\partial x^\mu}{\partial\sigma}\right)^2 - \left(\frac{\partial x^\mu}{\partial\tau}\right)^2\left(\frac{\partial x^\nu}{\partial\sigma}\right)^2\right], \tag{3.4}$$

where (σ, τ) are space and time coordinates on the surface of evolution of the string, and x^μ the space– time coordinates of a formal point particle on the string. Both I_1 and I_2 give the equations of motion of the string, but only the latter leads to the Virasoro gauge conditions necessary for the elimination of ghost states in the dual resonance model. Geometrically the stationary action I_2 defines a minimal surface, alternatively, and more rigorously, characterized by the vanishing of the mean curvature vector of the surface,[15–17] whilst the integrand in I_1 is also that which appears in the Dirichlet integral for harmonic analysis, and coincides (as a double integral) with the area integral I_2 in orthonormal coordinate systems, only.

For the characterization of minimal surfaces in terms of curvature, let N denote a surface (two-dimensional), and $x : N \to M$ be the immersion of N in M, where for the present paper M will be either space– time or a spacelike three-dimensional hypersurface, denoted $M^{(3)}$. The covariant derivative $D_u Y$ with respect to the Riemannian connection of M in a direction u tangential to N of any vector field Y normal to N can be decomposed into normal and tangential components by

$$D_u Y = \nabla_u Y - A^Y{}_{(u)}, \tag{3.5}$$

where ∇_u is the covariant derivative in the bundle of normal vectors to N, and $A^Y(u)$ is the second fundamental form on N. Using the Riemannian metric $g(X, Y)$ of M, a symmetric quadratic form $B(u, v)$ is defined on N by

$$g(B(u,v), Y) = g(A^Y(u), v), \tag{3.6}$$

where $u, v \in T(N)$, $Y \in T^\perp(N)$. The mean curvature vector H is then defined to be the trace of $B(u, v)$

$$H = \tfrac{1}{2} B_{\alpha\beta} g^{\alpha\beta}, \quad 1 \le \alpha, \beta \le 2, \tag{3.7}$$

where α, β are indices of coordinates on N. For the space– time applications two types of surface N will be considered: (1) those with indefinite metric, and (2) those with negative-definite metric.

The relation of minimal surfaces to geometric quantization is largely governed by the Weierstrass correspondence[15] between such surfaces and analytic functions, and also their connections with two-component spinors. Let $M^{(3)}$ denote a three-dimensional spatial hypersurface, then from the general existence of iso-

thermal parameters in two dimensions, the immersion $x: N \to M^{(3)}$ can be represented conformally, and x defined in terms of analytic functions on N. For the connection with geometric quantization, N must be chosen such that the decomposition

$$T_x(M) = T_x(N) \oplus T_x^{\perp}(N) \tag{3.8}$$

is preserved up to an orientation by J. Let $\{u_1, u_2\}$ be a basis for $T_x(N)$ and $\{w^1, w^2\}$ be the corresponding dual basis (i.e., 1-forms on N); then

$$\Delta x = -Hw^1 \wedge w^2, \tag{3.9}$$

where H is the mean curvature vector of the immersion $x: N \to M^{(3)}$, and Δ the Laplace–Beltrami operator on N. For a minimal surface $H = 0$, and the immersion is conformal (similarly for $x: N \to M$). Let $z = u_1 + iu_2$ be a complex parameter on N; then (3.9) with $H = 0$ can be expressed as

$$\frac{dZ}{dz} \cdot \frac{dZ}{dz} = 0, \tag{3.10}$$

where $x(u_1, u_2)$, being a harmonic function of two real variables, is, for a simply connected domain, the real part of a suitable analytic function $Z(z)$, and dZ/dz is evidently a null vector in three-dimensional space.

A null vector of 3-space can be expressed in terms of two regular functions (ξ^1, ξ^2):

$$\begin{aligned} \frac{dZ^1}{dz} &= (\xi^1)^2 - (\xi^2)^2, \\ \frac{dZ^2}{dz} &= i\{(\xi^1)^2 + (\xi^2)^2\}, \\ \frac{dZ^3}{dz} &= 2\xi^1\xi^2. \end{aligned} \tag{3.11}$$

According to the Cartan isotropic vector-spinor correspondence,[18] the two functions (ξ^1, ξ^2) constitute a spinor basis for SU(2). From (3.11) we get

$$\begin{aligned} x^1 &= \mathrm{Re} \int \{(\xi^1)^2 - (\xi^2)^2\} dz, \\ x^2 &= \mathrm{Re} \int i\{(\xi^1)^2 + (\xi^2)^2\} dz, \\ x^3 &= \mathrm{Re} \int 2\xi^1\xi^2 dz. \end{aligned} \tag{3.12}$$

The spinor basis (ξ^1, ξ^2) can be replaced by any regular function $f(\tau)$ of the complex variable τ defined by

$$\begin{aligned} \tau &= \xi^2/\xi^1, \\ f(\tau) &= (\xi^1)^4 / \left\{ \frac{d\xi^2}{dz}\xi^1 - \frac{d\xi^1}{dz}\xi^2 \right\}, \end{aligned} \tag{3.13}$$

thereby associating a minimal surface with any regular function of a complex variable.

From the Weierstrass relationships it follows that any minimal surface can be represented as a translation surface generated by null curves:

$$x(u_1, u_2) = y(u_1) + v(u_2), \tag{3.14}$$

where $y(u_1)$ and $v(u_2)$ are the null generators, from which a family of associated minimal surfaces $x(u_1, u_2, \theta)$ can be obtained by rotation in the yv plane

$$x(u_1, u_2, \theta) = e^{i\theta} y(u_1) + e^{-i\theta} v(u_2). \tag{3.15}$$

For minimal surfaces with indefinite metric, an analogous set of results holds,[19] and the generation by null curves indicates that the minimal surfaces in M are two-dimensional sections of the light cone; as the conformal structure is determined by J and a phase angle represented by a rotation in the $(u_0 \wedge u_3)$ and $(u_1 \wedge u_2)$ planes, the effect of the latter is to choose particular members of the family of minimal surfaces (3.15) for J.

In order to show how the strings of hadron physics may describe quark binding, we consider the generalized Gauss map[16,17] $\gamma: N \to G^{\mathbb{R}}(3,2)$ associated with the immersion $x: N \to M^{(3)}$ by $u \mapsto T_u(N)$, $u \in N$, where $G^{\mathbb{R}}(3,2)$ denotes the Grassmann space of real oriented 2-planes in three dimensions, and

$$G^{\mathbb{R}}(3,2) \approx \mathrm{SO}(3,\mathbb{R})/\mathrm{SO}(2) \times \mathrm{SO}(1). \tag{3.16}$$

The Weierstrass relationships permits the Grassmann space to be identified with the null quadric Q_1, that can be regarded as a subspace of the complex projective space $P_2(\mathbb{C})$, where

$$Q_1 = \{q = (q_1, q_2, q_3) \in P_2(\mathbb{C}) \mid \sum_{k=1}^{3} q_k^2 = 0\}. \tag{3.17}$$

The identification results from considering the action of the complexified group $\mathrm{SO}(3,\mathbb{C})$ on the vectors $\{q\} \in \mathbb{C}^3$, where q is the gradient dZ/dz of the immersion $x: N \to M^{(3)}$ in (3.9)–(3.11). The complexification $\mathrm{SO}(3,\mathbb{R}) \to \mathrm{SO}(3,\mathbb{C})$ is the result of regarding a harmonic function of two variables as the real part of an analytic function of a single complex variable with the complex structure induced by the restriction of J to $T(N)$.

It was suggested[1] that a point particle with energy – momentum vector p^μ would have $T^{\mu\nu}$ of type $[T - 3S]_{(2)}$ with $S = 0$, spin $\frac{1}{2}$ by the Cartan isotropic vector argument, and a symmetry group U(3) broken by the trace of $T^{\mu\nu}$, and hence might describe a baryon. The point particle of a hypersurface $M^{(3)}$ orthogonal to p^μ can be described nonlocally by the intersection of three planes, each of which defines an element of $G^{\mathbb{R}}(3,2)$, and by (3.17) also of $P_2(\mathbb{C})$ provided a suitable complex structure exists for each plane. This situation occurs if space–time admits an almost quaternionic structure whose $\mathrm{SO}(3,\mathbb{R})$ structure group realized by rotations in the space orthogonal to p^μ (which also defines the time-like eigenvector of $T^{\mu\nu}$). Each of the three almost complex structures J_a can be used to set up the Weierstrass formalism on the tangent space $T(N_a)$ $1 \le a \le 3$ spanned by the Ricci eigenvectors $V^b \wedge V^c$ $1 \le b, c \ne a \le 3$. Each of the resultant minimal immersions $x: N_a \to M^{(3)}$ has a gradient vector $q_a \equiv dZ/dz^a$, hence the point $x \in M^{(3)}$ is represented in $P_2(\mathbb{C})$ by the product of the three states, v_a. Each of these defines a basis vector of $\mathbb{C}^3$ and hence a formal quark state, which by (3.11) is also a formal spin $\frac{1}{2}$ object under $\mathrm{SO}(3,\mathbb{R})$. A transitive and effective group on $P_2(\mathbb{C})$ is $\mathrm{SU}(3)/Z_3$, with isotropy group U(2) leaving a single minimal surface invariant.

Since each oriented plane is defined by Ricci eigenvectors as $V^b \wedge V^c$ and defines a point of $P_2(\mathbb{C})$, it follows that the SU(3) group can be regarded as a subgroup of the generalized duality group U(3) for the trace-free tensor $U^{\mu\nu}$ of type $[T - 3S]_{(2)}$ with $V^b \wedge V^c$ isomorphous to a (1,0) symmetric spinor basis of U(3). If minimal

spatial surfaces are identified with strings, then a string model is obtained with three strings tied at one end, and for each quark the Hamiltonian h (see Sec. II) $=(T-S)x^a$, $1 \leq a \leq 3$ with x^a the displacement along the a-th string, and in this case $S=0$. The minimal surface /spinning string relationship is examined in the next section.

IV. MINIMAL SURFACES AND SUPERGAUGE THEORY

For minimal immersions $x: N \to M$ of spacelike surfaces, x satisfies (3.9) with $H=0$, i.e.,

$$\Delta x = 0 \tag{4.1}$$

the two-dimensional conformal equation on N. In isothermal coordinates Δ is given by $\partial^2/\partial u_1^2 + \partial^2/\partial u_2^2$ for spatial surfaces N, and for N with indefinite metric (4.1) is true with $\Delta \equiv \partial^2/\partial u_0^2 - \partial^2/\partial u_3^2$. As in each case x is normal to the surface N, it transforms as a scalar under the conformal transformations of N. The gradient dZ/dz of the immersion defines a null vector for $x: N \to M$[3] and hence a two-component spinor, φ, which as the gradient of x, satisfies a first order equation

$$\gamma^a \frac{\partial}{\partial u_\alpha}\varphi = 0, \tag{4.2}$$

where γ^α are the two-dimensional gamma matrices

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

for Minkowski surfaces and

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

for spacelike surfaces. In this, the situation is similar to basic string theory,[8] but for immersions $x: N \to M$ a major difference occurs as the spinor φ has to be replaced by a null vector ψ of the 4-geometry, i.e., must define a photon state.

Solutions of (4.1) and (4.2) proceed as in elementary string theory, except that in the case of spacelike minimal surfaces the eigenvalues of the exponentials in u_1 and u_2 must be opposite in sign

$$x^\mu = x^\mu(0) + p^\mu(0)u^2 + \sum_{n=0}^{\infty} x_n^\mu \cos n u^1 \exp(-inu^2), \tag{4.3}$$

where $x^\mu(0)$ and $p^\mu(0)$ are constants of integration, and unlike the string models no boundary conditions have been specified. As a minimal surface is the generalization to curved space of a plane in the same way as geodesics are related to straight lines, the open string conditions seem more appropriate, but with closed string conditions relevant in black hole physics.

Constraints arise from the requirement of conformal invariance in two dimensions, where instead of the full conformal group being of second order an infinite parameter group[10] is generated by the elements

$$X = \sum_{\alpha=1}^{2} f^\alpha(u)\partial/\partial u^\alpha,$$

where $f^\alpha(u)$ is an arbitrary function on N. Expressing the minimal Minkowski surface coordinates in the light-cone form

$$u_\pm = (1/\sqrt{2})(u_0 \pm u_3) \tag{4.4}$$

the infinitesimal operators of the full conformal group can be expressed as

$$C_{n\pm} = i(u_\pm)^n \partial^\pm, \tag{4.5}$$

where

$$\partial^\pm = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial u_0} \pm \frac{\partial}{\partial u_3}\right) \tag{4.6}$$

which satisfy the commutation relations

$$[C_{n\alpha}, C_{m\beta}] = i\delta_{\alpha\beta}(m-n)C_{m+n-1,\alpha}, \tag{4.7}$$

where $\alpha, \beta \in \{+,-\}$ and (4.7) is not summed over α. Of the set $\{C_{n\pm}\}$ the subset $\{C_{0\pm}, C_{1\pm}, C_{2\pm}\}$ generates, respectively, the translations, Lorentz rotation and dilatation, and the special conformal transformations. In this minimal surface approach the infinite set of classical Virasoro constraints is replaced by the infinite set of constraints corresponding to invariance under transformations generated by $\{C_{n\pm}\}$.

For the supergauge transformation of the Ramond – Neveu – Schwarz model[20–22] given by

$$\begin{aligned} &\delta x = i\bar{\alpha}\varphi, \\ &\delta\varphi = \partial_i x \gamma^i \alpha + F\alpha, \\ &\delta F = i\bar{\alpha}\gamma^i \partial_i \varphi, \quad 1 \leq i \leq 2, \end{aligned} \tag{4.8}$$

where α is an anticommuting parameter, to be permissible they must preserve the functional relationship that exists between x and φ for minimal immersions. This relationship can be expressed in the general form

$$x^\mu = \mathrm{Re}\int \gamma^\mu_{ab}\varphi^a\varphi^b\, dz, \quad 1 \leq a \leq 2 \tag{4.9}$$

so that in addition to the usual spatial transformations of x^μ there are further degrees of freedom associated with the complexified rotations, and in principle a purely imaginary translation δx could be expressed in the spinorial form of (4.8), provided the overall set of transformations were compatible with the conformal invariance in two dimensions required of a minimal immersion, and the usual set of transformations (4.8) do achieve this when the parameter α satisfies a two-dimensional conformal equation of motion.

According to the geometric quantization vectors and spinors must be quantized[3] according to

$$[x^\mu, x^\nu] = ig(x^\mu, Jx^\nu) \tag{4.10}$$

$$\{\psi^\mu, \psi^\nu\} = 2g^{\mu\nu} \tag{4.11}$$

in the Segal type of scheme, or in the generally inequivalent Kostant representation $g(x^\mu, Jx^\nu)$ in (4.10) is replaced by the Ricci form $R(x^\mu, Jx^\nu)$. If the string coordinates x^μ are quantized in this way, then the expansion coefficients x_n^μ in (4.3) must also be quantized. If the commutation relations $[x_n^\mu, x_m^{\nu\dagger}] = g^{\mu\nu}\delta_{mn}$ are to be compatible with the Kostant quantization of harmonic oscillations of the geometry in Sec. II, then the expansion coefficients must be rescaled by a parameter $\sqrt{2\alpha'}$ such that $2\alpha' = \frac{1}{4}R$ for an Einstein space, or $\alpha'_{03} = \frac{1}{2}(T - S_3)$ and $\alpha'_{12} = \frac{1}{2}(S_1 + S_2)$ for the 0–3 and 1–2 planes in the non-Einstein case $[T - S_1 - S_2 - S_3]_{(4)}$, where in dual

resonance models α' is interpreted as the slope of the Regge trajectory.

It seems natural also to try to define pure gravity, i.e., the conformal structure (J, θ), in terms of the string formalism by specifying minimal surfaces. Let $T(M) = T(N) \oplus T^{\perp}(N)$ be a decomposition of the tangent space of M, and this time require both N and $N^{\perp}$ to be minimally immersed in M. The immersion $x : N^{\perp} \to M$ defines a null vector dZ/dz_1, where z_1 is a complex parameter on N and $x = \mathrm{Re} \int (dZ/dz_1)\, dz_1$ is normal to N, i.e., lies in $T^{\perp}(N)$. Similarly, the immersion $x : N^{\perp} \to M$ defines another null vector dZ/dz_2, where $z_1 = u_1 + iu_2$, $z_2 = u_0 + u_3$, where u^i are coordinates on $N, N^{\perp}$; and x satisfies both

$$\frac{\partial^2 x}{(\partial u_1)^2} + \frac{\partial^2 x}{(\partial u_2)^2} = 0 \quad \text{and} \quad \frac{\partial^2 x}{(\partial u_0)^2} - \frac{\partial^2 x}{(\partial u_3)^2} = 0$$

and hence satisfies the zero mass Klein–Gordon equation in space–time. Considering again the generalized Gauss maps, the minimal surfaces N and $N^{\perp}$ are each associated with elements dZ/dz of the quadric Q_2 in $P^3(\mathbb{C})$ on which the complexified rotation group $SO(4, \mathbb{C})$ acts. Both dZ/dz_1 and dZ/dz_2 must define spinors of the two-dimensional conformal group on the surfaces N and $N^{\perp}$, but the choice of these surfaces is arbitrary apart from the J-conjugacy, and must be made Lorentz covariant. For Lorentz covariance of the pair of minimal immersions, dZ/dz_1 and dZ/dz_2 must define a single spinor representation of the full conformal group of spacetime, i.e., a twistor[23] representation of SU(2, 2).

V. DISCUSSION

This paper shows that a large part of the formalism of contemporary theoretical physics can be described in a purely geometric context, and since geometric and representation theoretic concepts are already implicit in field theory no extra physical assumption is involved in applying the more obscure geometric ideas to physics also, although there is no a priori guarantee of their relevance at scales of distance and energy involved in presently observable phenomena. If the identifications with formally similar physical phenomena are taken seriously, it means that:

(1) strings are minimal surfaces with either negative definite, or indefinite metric;

(2) quarks are the gradients of minimal immersions of spacelike surfaces in three-dimensional spatial hypersurfaces;

(3) baryons are point particles of three-dimensional spatial hypersurfaces with $T^{\mu\nu}$ of type $[T - 3S]_{(2)}$, consisting of three quarks bound together in the internal space $P^2(\mathbb{C})$ by three spacelike strings, and

(4) the slopes of Regge trajectories are determined by the eigenvalues of the Ricci tensor.

Physically the interpretation (1) is obviously not necessary since strings of vortices, thin compared to their length, have been shown to give surfaces of minimal area via the transverse Lorentz contraction factor in the Lagrangian,[24] whilst the successes of the colour gluon model provide an alternative to (3). A lot of geometric concepts of relevance to constraints have been omitted from consideration here; in particular, the maximal immersion[25,26] of three-dimensional hypersurfaces in space–time required for positive gravitational energy, and the definition of spinning strings and supergravity via the square root of the Hamiltonian constraints,[27,28] and all of these are required for consistent propagation of the fields. The real drawback of the geometric approach to quarks is that whilst it does not appear to require color, it cannot explain all five currently known quark flavors.

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Polynomial tensors for double point groups[a)]

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Generating functions for (Γ_r,Γ_m) tensors for each pair of irreducible representations Γ_r and Γ_m are calculated for each double point group. A (Γ_r,Γ_m) tensor transforms according to Γ_r and its components are polynomials in another tensor transforming by Γ_m. The actual tensors are given for the groups ${}^{(d)}C_n$, ${}^{(d)}D_n$, ${}^{(d)}T$ and for some representations Γ_m of ${}^{(d)}O$. Certain of the polynomial tensors provide polynomial SU(2) bases reduced according to the double point group in question.

I. INTRODUCTION

In a recent paper[1] (to be referred to as I), generating functions are given for the point groups C_n, D_n, T, O, and I (and for point groups involving reflections) for Γ_r, Γ_m) tensors transforming by a particular irreducible representation (IR) Γ_r whose components are polynomials in the components of a tensor transforming by another IR Γ_m; for C_n, D_n, T and O the explicit polynomials are given.

In this paper we carry out similar calculations for the double point groups. In Sec. 2 the generating functions are given for each of ${}^{(d)}C_n$, ${}^{(d)}D_n$, ${}^{(d)}T$, ${}^{(d)}O$, and ${}^{(d)}I$. Section 3 contains integrity bases which yield directly the explicit polynomial tensors for ${}^{(d)}C_n$, ${}^{(d)}D_n$, ${}^{(d)}T$ and for some IR's Γ_m of ${}^{(d)}O$. In Sec. 4 we outline the use of certain of the tensors as polynomial bases for SU(2), reduced according to a double point group [or O(3) reduced according to the corresponding point group].

The remainder of this section is devoted to a review of general properties and the method of calculation of the generating functions. A somewhat complete bibliography of the subject is found in I.

The generating function $B_{r,m}(\lambda)$ carries important information about (Γ_r,Γ_m) tensors. If $B_{r,m}(\lambda)$ is expanded in powers of λ,

$$B_{r,m}(\lambda)=\sum_p c_p\lambda^p, \tag{1}$$

then c_p is the number of linearly independent (Γ_r, Γ_m) tensors of degree p. $B_{r,m}(\lambda)$ may be calculated from the formula[2]

$$B_{r,m}(\lambda)=\frac{1}{N}\sum_s \frac{N_s\chi^*_{sr}}{\det(1-\lambda A_s)}. \tag{2}$$

Here N is the order of the group G, N_s is the order of the the class s, χ_{sr} is the character of s for Γ_r, and A_s is the matrix which represents some element of s in Γ_m.

In all our examples $B_{r,m}(\lambda)$ may be written in the form

$$B_{r,m}(\lambda)=(\sum_p k_p\lambda^p)/\prod_q(1-\lambda^q)^{l_q}, \tag{3}$$

where the sum and product are finite. To each denominator factor $1-\lambda^q$ corresponds a functionally independent scalar of degree q in the components of the Γ_m tensor. The number $\sum_q l_q$ of such scalars is the dimension f_m of the IR Γ_m. Each numerator term $k_p\lambda^p$ implies the existence of k_p linearly independent (Γ_r, Γ_m) tensors of degree p (they are also linearly independent of any lower degree Γ_r tensor multiplied by denominator scalars).

A useful check on the correctness of the generating function is the dimensionality condition[1]

$$\sum_r f_r B_{r,m}(\lambda)=(1-\lambda)^{-f_m}; \tag{4}$$

f_r is the dimension of Γ_r.

The following composition rule[1] is useful for constructing a generating function for Γ_r tensors which are polynomials in the components of two tensors transforming by Γ_m and $\Gamma_{m'}$ [$(\Gamma_r,\Gamma_m+\Gamma_{m'})$ tensors]:

$$B_{r;m,m'}(\lambda,\lambda')=\sum_{r',r''} B_{r',m}(\lambda)B_{r'',m'}(\lambda')C_r^{r'r''}, \tag{5}$$

where $C_r^{r'r''}$ is the multiplicity of Γ_r in the direct product $\Gamma_{r'}\otimes\Gamma_{r''}$.

2. GENERATING FUNCTIONS FOR DOUBLE POINT GROUP TENSORS

A double point group ${}^{(d)}G$ is a subgroup of SU(2) just as the corresponding point (finite rotation) group G is a subgroup of SO(3). To get the defining matrix representation of the double group, write down the (rotation) matrices for the $j=\frac{1}{2}$ representation of SU(2) which represent the rotations of the point group.[3] Since each element appears with its negative, ${}^{(d)}G$ has twice as many elements as G. It may not have twice as many classes (and IR's) however, since elements with zero character (180° rotations) may fall into the same class as their negatives.

The IR's of the double point group ${}^{(d)}G$ may be classified as odd and even. The odd IR's are found in the reduction of half-odd IR's of SU(2) while even IR's are found in integer IR's of SU(2). Even IR's of ${}^{(d)}G$ correspond one-to-one to IR's of G. The matrices which represent an element and its negative, for an even IR, are both equal to the matrix which represents the corresponding rotation for the corresponding IR of G.

It follows from Eq. (2) that the generating function $B_{r,m}(\lambda)$, where Γ_r and Γ_m are both even IR's of the double point group ${}^{(d)}G$, is equal to the generating function $B_{r,m}(\lambda)$, where Γ_r and Γ_m are the corresponding IR's of G. If Γ_r is an odd IR and Γ_m an even IR of ${}^{(d)}G$, then

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$B_{r,m}(\lambda)=0$. Hence we present in this section only those generating functions $B_{r,m}(\lambda)$ (and in the next section only those invariants and tensors I_m and $E_{r,m}$) for which Γ_m is an odd IR. The generating functions and tensors with Γ_m even are found in Ref. 1. For Γ_m odd, $B_{r,m}(\lambda)$ is an even (odd) function of λ if Γ_r is an even (odd) IR; even tensors are of even degree, odd tensors of odd degree, in the components of an odd tensor.

A. The group ${}^{(d)}C_n$

The group ${}^{(d)}C_n$ corresponds to the group C_n of rotations about an nth order axis. ${}^{(d)}C_n$ is isomorphic[3] to C_{2n}; thus it has $2n$ classes and $2n$ IR's. The generating functions are given by I, Eq. (15): (here Γ_m can be odd or even):

$$B_{r,m}(\lambda)=\lambda^p(1-\lambda^a)^{-1}, \tag{6}$$

where

$$\begin{aligned} &a=2n/\mathrm{HCF}(2n, m-1),\\ &r=p(m-1)_{\mathrm{mod}\,2n}+1, \quad 0\le p\le a-1. \end{aligned} \tag{7}$$

HCF means highest common factor. The even (or odd) IR's of ${}^{(d)}C_n$ are the IR's Γ_m of C_{2n} for which m is odd (or even). The even IR Γ_{2m-1} of ${}^{(d)}C_n$ corresponds to the IR Γ_m of C_n $(1\le m\le n)$.

B. The group ${}^{(d)}D_n$

${}^{(d)}D_n$ corresponds to the group D_n of rotations about an nth order vertical axis and n horizontal second order axes. It closely resembles in structure the group D_{2n}. The two groups have the same number of classes and IR's, $n+3$; they differ only in that, for odd IR's of ${}^{(d)}D_n$, the matrices of the two classes which, for D_{2n}, contain rotations π about horizontal axes, contain an additional factor i. The odd IR's are those two dimensional Γ_m for which m is odd, for n odd only, the one-dimensional IR's Γ_3 and Γ_4. For n odd the even IR's Γ_1 and Γ_2 of ${}^{(d)}D_n$ correspond to the IR's Γ_1 and Γ_2 of D; the even IR Γ_{2m} of ${}^{(d)}D_n$ corresponds to Γ_m of D_n $[3\le m\le (n+3)/2]$. For n even the even IR's Γ_1, Γ_2, Γ_3, Γ_4 of ${}^{(d)}D_n$ correspond to the same IR's of D_n while the even IR Γ_{2m} of ${}^{(d)}D_n$ corresponds to Γ_{m+2} of D_n $(3\le m\le \frac{1}{2}n+1)$.

For ${}^{(d)}D_n$, the polynomials $\det(1-\lambda A_s)$ are given in Table I. With their help we find the generating functions $B_{r,m}(\lambda)$ for odd IR's Γ_m.

When n is odd, Γ_3 and Γ_4 are odd, and we obtain

$$\begin{aligned} &B_{1,3}(\lambda)=B_{1,4}(\lambda)=(1-\lambda^4)^{-1},\\ &B_{2,3}(\lambda)=B_{2,4}(\lambda)=\lambda^2(1-\lambda^4)^{-1},\\ &B_{3,3}(\lambda)=B_{4,4}(\lambda)=\lambda(1-\lambda^4)^{-1},\\ &B_{4,3}(\lambda)=B_{3,4}(\lambda)=\lambda^3(1-\lambda^4)^{-1}. \end{aligned} \tag{8}$$

For $5\le m\le n+3$, m odd, we get (when m is odd, a is even and $a/2$ has the parity of n)

$$\begin{aligned} &B_{1,m}(\lambda)=(1+\lambda^{a+2})[(1-\lambda^4)(1-\lambda^a)]^{-1},\\ &B_{2,m}(\lambda)=(\lambda^2+\lambda^a)[(1-\lambda^4)(1-\lambda^a)]^{-1},\\ &B_{3,m}(\lambda)=B_{4,m}(\lambda)=(\lambda^{a/2}+\lambda^{a/2+2})[(1-\lambda^4)(1-\lambda^a)]^{-1},\\ &B_{r,m}(\lambda)=(\lambda^p+\lambda^{p+2}+\lambda^{a-p}+\lambda^{a-p+2})[(1-\lambda^4)(1-\lambda^a)]^{-1}. \end{aligned} \tag{9}$$

In Eq. (9), a and p are related to m and r by

$$\begin{aligned} &a=2n/\mathrm{HCF}\,(2n, m-4),\\ &r=n-\left|p(m-4)_{\mathrm{mod}\,2n}-n\right|+4; \end{aligned} \tag{10}$$

p takes the values $1, 2, \ldots, \frac{1}{2}a-1$.

C. The groups ${}^{(d)}$T, ${}^{(d)}$O, and ${}^{(d)}$I

The groups ${}^{(d)}T$, ${}^{(d)}O$, and ${}^{(d)}I$ are the double groups which correspond to the point groups T (tetrahedral), O (octahedral), and I (icosahedral). The polynomials $\det(1-\lambda A_s)$ for these double groups are given in Tables II, III, and IV respectively. The characters also may be read from these tables; they are the coefficients λ, with sign reversed. We have given the even IR's the same numbers as the corresponding IR's of the corresponding point group in Ref. 1. ${}^{(d)}T$ has four even IR's and three odd; ${}^{(d)}O$ has five even and three odd; ${}^{(d)}I$ has five even and four odd.

The generating functions $B_{r,m}(\lambda)$, where Γ_m is an odd IR of ${}^{(d)}T$, ${}^{(d)}O$, or ${}^{(d)}I$ are given in Tables V, VI, VII respectively. Recall the form (3) of the generating function. A term $k_p\lambda^p$ in the numerator of $B_{rm}(\lambda)$ is indicated by an entry $p^k{}_p$ in the Γ_m row, Γ_r column of the table. A factor $(1-\lambda^q)^{lq}$ in the denominator is indicated by an entry q^{lq} in the Γ_m row, denominator column (all generating functions based on Γ_m have the same denominator). For example we read from Table VII (group ${}^{(d)}I$)

TABLE I. Polynomials $\det(1-\lambda A_s)$ for the double group ${}^{(d)}D_n$, n odd. For n even, the following changes should be made for IR's Γ_3 and Γ_4: for the class A^n, the polynomial $1+\lambda$ should be $1-\lambda$, and for classes B and AB, $i\lambda$ in the polynomials should be replaced by λ.

N_s	1	1	2	n	n
IR \ Class	I	A^n	A^s, A^{2n-s} $(s=1, 2, \ldots, n-1)$	B	AB
Γ_1	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$
Γ_2	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1+\lambda$	$1+\lambda$
Γ_3	$1-\lambda$	$1+\lambda$	$1-(-1)^s\lambda$	$1-i\lambda$	$1+i\lambda$
Γ_4	$1-\lambda$	$1+\lambda$	$1-(-1)^s\lambda$	$1+i\lambda$	$1-i\lambda$
Γ_r $(r=5, 7, \cdots)$	$(1-\lambda)^2$	$(1+\lambda)^2$	$1-2\lambda\cos\{\pi(r-4)\,s/n\}+\lambda^2$	$1+\lambda^2$	$1+\lambda^2$
Γ_r $(r=6, 8, \cdots)$	$(1-\lambda)^2$	$(1-\lambda)^2$	$1-2\lambda\cos\{\pi(r-4)\,s/n\}+\lambda^2$	$1-\lambda^2$	$1-\lambda^2$

TABLE II. Polynomials $\det(1-\lambda A_s)$ for the double tetrahedral group; $\omega=\exp(2\pi i/3)$.

N_s	1	1	6	4	4	4	4
IR \ Class	I	R	C_2	C_3	C_3'	C_4	C_4'
Γ_1	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$
Γ_2	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\omega\lambda$	$1-\omega\lambda$	$1-\omega^2\lambda$	$1-\omega^2\lambda$
Γ_3	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\omega^2\lambda$	$1-\omega^2\lambda$	$1-\omega\lambda$	$1-\omega\lambda$
Γ_4	$(1-\lambda)^3$	$(1-\lambda)^3$	$(1-\lambda)(1+\lambda)^2$	$1-\lambda^3$	$1-\lambda^3$	$1-\lambda^3$	$1-\lambda^3$
Γ_5	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\lambda^2$	$1-\lambda+\lambda^2$	$1+\lambda+\lambda^2$	$1+\lambda+\lambda^2$	$1-\lambda+\lambda^2$
Γ_6	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\lambda^2$	$1-\omega\lambda+\omega^2\lambda^2$	$1+\omega\lambda+\omega^2\lambda^2$	$1+\omega^2\lambda+\omega\lambda^2$	$1-\omega^2\lambda+\omega\lambda^2$
Γ_7	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\lambda^2$	$1-\omega^2\lambda+\omega\lambda^2$	$1+\omega^2\lambda+\omega\lambda^2$	$1+\omega\lambda+\omega^2\lambda^2$	$1-\omega\lambda+\omega^2\lambda^2$

$$B_{7,8}(\lambda)=(\lambda^5+3\lambda^7+4\lambda^9+4\lambda^{11}+3\lambda^{13}+\lambda^{15})/(1-\lambda^4)^2(1-\lambda^6)\times(1-\lambda^{10}).$$

3. INTEGRITY BASES FOR DOUBLE POINT GROUP POLYNOMIAL TENSORS

The form (3) of the generating function $B_{r,m}(\lambda)$ indicates that the most general (Γ_r, Γ_m) tensor can be expressed in terms of a finite number of "elementary" (Γ_r, Γ_m) tensors $E^{(p)}_{r,m}$ corresponding to the terms λ^p in the numerator of $B_{r,m}(\lambda)$ and a finite number of elementary scalars $I^{(q)}_m$ which correspond to the denominator factors $1-\lambda^q$. The degree of the elementary tensor or scalar is the exponent of λ in each case. The elementary tensors $E^{(p)}_{r,m}$ are said to form an integrity basis for the general (Γ_r, Γ_m) tensor, which is a linear combination of $E^{(p)}_{r,m}$ with coefficients which are polynomials in the scalars $I^{(q)}_m$. In particular $E^{(p)}_{1,m}$ is the scalar which corresponds to the term λ^p in the numerator of $B_{1,m}(\lambda)$.

To determine an elementary (Γ_r, Γ_m) tensor, let its components be arbitrary polynomials of the required degree in the components of the Γ_m tensor and ask that it be transformed by Γ_r when the components on which it depends are transformed by Γ_m. For this purpose it is necessary to apply only the generating elements of the group. The explicit generating matrices we use for odd IR's of dimension greater than one are given in Table VIII; those for even IR's are found in I. For a one-dimensional IR the matrix is the character. When there is more than one (Γ_r, Γ_m) tensor of a particular degree, the additional criteria of linear independence and (hopefully) simplicity must be invoked.

We give below the results of our computation of the scalars $I^{(q)}_m$ and tensors $E^{(p)}_{r,m}$, with Γ_m odd, for the double groups ${}^{(d)}C_n$, ${}^{(d)}D_n$, ${}^{(d)}T$, and some cases of ${}^{(d)}O$. The superscript p or q may be omitted where no confusion can arise, or an additional subscript may be affixed to distinguish two elementary tensors of the same degree.

The components of the Γ_m tensor are denoted by $\alpha, \beta, \gamma, \cdots$, and correspond to the rows 1, 2, 3, $\cdots$ of the generating matrices in Table VIII.

A. ${}^{(d)}C_n$ tensors

Since ${}^{(d)}C_n$ is isomorphic to C_{2n}, the tensors are those given by Eq. (40) of I:

$$I_1=\alpha,\quad I_m=\alpha^a,\quad E_{r,m}=\alpha^p. \tag{11}$$

a and p are defined by Eq. (7). Γ_m is not restricted to odd IR's.

B. ${}^{(d)}D_n$ tensors

For n odd, the IR's Γ_3 and Γ_4 are odd. The elementary scalars and tensors based on Γ_3 or Γ_4 tensors are then

TABLE III. Polynomials $\det(1-\lambda A_s)$ for the double octahedral group.

N_s	1	1	6	6	6	12	8	8
IR \ Class	C_1	C_1'	C_2	C_3	C_3'	C_4	C_5	C_5'
Γ_1	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$
Γ_2	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1+\lambda$	$1+\lambda$	$1+\lambda$	$1-\lambda$	$1-\lambda$
Γ_3	$(1-\lambda)^2$	$(1-\lambda)^2$	$(1-\lambda)^2$	$1-\lambda^2$	$1-\lambda^2$	$1-\lambda^2$	$1+\lambda+\lambda^2$	$1+\lambda+\lambda^2$
Γ_4	$(1-\lambda)^3$	$(1-\lambda)^3$	$(1-\lambda)(1+\lambda)^2$	$(1+\lambda)(1+\lambda^2)$	$(1+\lambda)(1+\lambda^2)$	$(1-\lambda)^2(1+\lambda)$	$1-\lambda^3$	$1-\lambda^3$
Γ_5	$(1-\lambda)^3$	$(1-\lambda)^3$	$(1-\lambda)(1+\lambda)^2$	$(1-\lambda)(1+\lambda^2)$	$(1-\lambda)(1+\lambda^2)$	$(1-\lambda)(1+\lambda)^2$	$1-\lambda^3$	$1-\lambda^3$
Γ_6	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\lambda^2$	$1-\sqrt{2}\lambda+\lambda^2$	$1+\sqrt{2}\lambda+\lambda^2$	$1+\lambda^2$	$1+\lambda+\lambda^2$	$1-\lambda+\lambda^2$
Γ_7	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\lambda^2$	$1+\sqrt{2}\lambda+\lambda^2$	$1-\sqrt{2}\lambda+\lambda^2$	$1+\lambda^2$	$1+\lambda+\lambda^2$	$1-\lambda+\lambda^2$
Γ_8	$(1-\lambda)^4$	$(1+\lambda)^4$	$(1+\lambda^2)^2$	$1+\lambda^4$	$1+\lambda^4$	$(1+\lambda^2)^2$	$(1-\lambda)(1-\lambda^3)$	$(1+\lambda)(1+\lambda^3)$

TABLE IV. Polynomials $\det(1-\lambda A_s)$ for the double icosahedral group $\kappa=\frac{1}{2}(1+\sqrt{5})$, $\bar{\kappa}=\frac{1}{2}(1-\sqrt{5})$.

N_s	1	1	12	12	12	12	30	20	20
IR \ Class	C_1	C_1'	C_2	C_2'	C_3	C_3'	C_4	C_5	C_5'
Γ_1	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$	$1-\lambda$
Γ_2	$(1-\lambda)^3$	$(1-\lambda)^3$	$(1-\lambda)(1+\kappa\lambda+\lambda^2)$	$(1-\lambda)(1+\bar{\kappa}\lambda+\lambda^2)$	$(1-\lambda)(1+\bar{\kappa}\lambda+\lambda^2)$	$(1-\lambda)(1+\kappa\lambda+\lambda^2)$	$(1-\lambda)(1+\lambda)^2$	$1-\lambda^3$	$1-\lambda^3$
Γ_3	$(1-\lambda)^3$	$(1-\lambda)^3$	$(1-\lambda)(1+\bar{\kappa}\lambda+\lambda^2)$	$(1-\lambda)(1+\kappa\lambda+\lambda^2)$	$(1-\lambda)(1+\kappa\lambda+\lambda^2)$	$(1-\lambda)(1-\kappa\lambda+\lambda^2)$	$(1-\lambda)(1+\lambda)^2$	$1-\lambda^3$	$1-\lambda^3$
Γ_4	$(1-\lambda)^4$	$(1-\lambda)^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$(1-\lambda^2)^2$	$(1-\lambda)(1-\lambda^3)$	$(1-\lambda)(1-\lambda^3)$
Γ_5	$(1-\lambda)^5$	$(1-\lambda)^5$	$1-\lambda^5$	$1-\lambda^5$	$1-\lambda^5$	$1-\lambda^5$	$(1-\lambda)^3(1+\lambda)^2$	$(1-\lambda)(1+\lambda+\lambda^2)^2$	$(1-\lambda)(1+\lambda+\lambda^2)^2$
Γ_6	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\bar{\kappa}\lambda+\lambda^2$	$1-\bar{\kappa}\lambda+\lambda^2$	$1+\kappa\lambda+\lambda^2$	$1-\kappa\lambda+\lambda^2$	$1+\lambda^2$	$1+\lambda+\lambda^2$	$1-\lambda+\lambda^2$
Γ_7	$(1-\lambda)^2$	$(1+\lambda)^2$	$1+\kappa\lambda+\lambda^2$	$1-\kappa\lambda+\lambda^2$	$1+\bar{\kappa}\lambda+\lambda^2$	$1-\bar{\kappa}\lambda+\lambda^2$	$1+\lambda^2$	$1+\lambda+\lambda^2$	$1-\lambda+\lambda^2$
Γ_8	$(1-\lambda)^4$	$(1+\lambda)^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$1-\lambda+\lambda^2-\lambda^3+\lambda^4$	$1+\lambda+\lambda^2+\lambda^3+\lambda^4$	$1-\lambda+\lambda^2-\lambda^3+\lambda^4$	$(1+\lambda^2)^2$	$(1-\lambda)(1-\lambda^3)$	$(1+\lambda)(1+\lambda^3)$
Γ_9	$(1-\lambda)^6$	$(1+\lambda)^6$	$(1-\lambda)(1-\lambda^5)$	$(1+\lambda)(1+\lambda^5)$	$(1-\lambda)(1-\lambda^5)$	$(1+\lambda)(1+\lambda^5)$	$(1+\lambda^2)^3$	$(1-\lambda^3)^2$	$(1+\lambda^3)^2$

$$I_3=I_4=\alpha^4,\quad E_{2,3}=E_{2,4}=\alpha^2,$$
$$E_{3,3}=E_{4,4}=\alpha,\quad E_{3,4}=E_{4,3}=\alpha^3. \tag{12}$$

We next give the elementary scalars and tensors based on Γ_m tensors, $5\le m\le n+3$, m odd. a and p are related to m and r by Eq. (10); a is even, and $\frac{1}{2}a$ has the parity of n. $[x]$ denotes the largest integer which does not exceed x.

$$I_m^{(4)}=\alpha^2\beta^2,\quad I_m^{(a)}=\alpha^a+(-1)^n\beta^a,$$
$$E_1^{(a+2)}=\alpha\beta[\alpha^a-(-1)^n\beta^a],$$
$$E_{2,m}^{(2)}=\alpha\beta,\quad E_{2,m}^{(a)}=\alpha^a-(-1)^n\beta^a,$$
$$E_{3,m}^{(a/2)}=\alpha^{a/2}+(-1)^{[a/4]}\beta^{a/2},$$
$$E_{3,m}^{(a/2+2)}=\alpha\beta[\alpha^{a/2}-(-1)^{[a/4]}\beta^{a/2}],$$
$$E_{4,m}^{(a/2)}=\alpha^{a/2}-(-1)^{[a/4]}\beta^{a/2},$$
$$E_{4,m}^{(a/2+2)}=\alpha\beta(\alpha^{a/2}+(-1)^{a/4}\beta^{a/2}),$$
$$E_{r,m}^{(p)}=\begin{cases}\left(\dfrac{\alpha^p}{(-1)^{[p/2]}\beta^p}\right), & 1\le\kappa\le n-1,\\[2ex] \left(\dfrac{\beta^p}{(-1)^{[p/2]}\alpha^p}\right), & n+1\le\kappa\le 2n-2,\end{cases}$$
$$E_{r,m}^{(p+2)}=\begin{cases}\alpha\beta\left(\dfrac{\alpha^p}{-(-1)^{[p/2]}\beta^p}\right), & 1\le\kappa\le n-1,\\[2ex] \alpha\beta\left(\dfrac{\beta^p}{-(-1)^{[p/2]}\alpha^p}\right), & n+1\le\kappa\le 2n-2,\end{cases}$$
$$E_{r,m}^{(a-p)}=\begin{cases}\left(\dfrac{\beta^{a-p}}{(-1)^{[(p+1)/2]+n}\alpha^{a-p}}\right), & 1\le\kappa\le n-1,\\[2ex] \left(\dfrac{\alpha^{a-p}}{(-1)^{[(p+1)/2]+n}\beta^{a-p}}\right), & n+1\le\kappa\le 2n-2,\end{cases} \tag{17}$$
$$E_{r,m}^{(a-p+2)}=\begin{cases}\alpha\beta\left(\dfrac{\beta^{a-p}}{(-1)^{[(p-1)/2]+n}\alpha^{a-p}}\right), & 1\le\kappa\le n-1,\\[2ex] \alpha\beta\left(\dfrac{\alpha^{a-p}}{(-1)^{[(p-1)/2]+n}\beta^{a-p}}\right), & n+1\le\kappa\le 2n-2,\end{cases}$$

where

$$\kappa=p(m-4)_{\text{mod }2n}. \tag{18}$$

C. $^{(d)}T$ tensors

The degrees of the scalars and tensors based on the odd IR's, Γ_5, Γ_6, Γ_7, of $^{(d)}T$ may be read from Table VI.

For the elementary scalars we find

$$I_5^{(6)}=\alpha^5\beta-\alpha\beta^5,\quad I_5^{(8)}=\alpha^8+14\alpha^4\beta^4+\beta^8,$$
$$I_6^{(4)}=I_7^{(4)*}=\alpha^4-2i\sqrt{3}\alpha^2\beta^2+\beta^4$$
$$I_6^{(6)}=I_7^{(6)}=\alpha\beta(\alpha^4-\beta^4), \tag{15}$$
$$E_{1,5}^{(12)}=(\alpha^4+\beta^4)(\alpha^8-34\alpha^4\beta^4+\beta^8).$$

The other elementary tensors based on Γ_5 are

$$E_{2,5}^{(4)}=\alpha^4+2\sqrt{3}\,i\alpha^2\beta^2+\beta^4,$$
$$E_{2,5}^{(8)}=\alpha^8-4\sqrt{3}\,i\alpha^6\beta^2-10\alpha^4\beta^4-4\sqrt{3}\,i\alpha^2\beta^6+\beta^8,$$
$$E_{3,5}^{(4)}=\alpha^4-2\sqrt{3}\,i\alpha^2\beta^2+\beta^4,$$

TABLE V. Generating functions for tensors based on odd IR's of the double tetrahedral group.

Γ_m \ Γ_r	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Denom.
Γ_5	0, 12	4, 8	4, 8	2, 4, 6^2, 8, 10	1, 5, 7, 11	3, 5, 7, 9	3, 5, 7, 9	6, 8
Γ_6	0	8	4	2, 4, 6	5, 7	1, 3	3, 5	4, 6
Γ_7	0	4	8	2, 4, 6	5, 7	3, 5	1, 3	4, 6

TABLE VI. Generating functions for tensors based on odd IR's of the double octahedral group.

Γ_m \ Γ_r	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Denom.
Γ_6	0, 18	6, 12	4, 8, 10, 14	2, 6, 8, 10, 12, 16	4, 6, 8, 10, 12, 14	1, 7, 11, 17	5, 7, 11, 13	3, 5, 7, 9^2, 11, 13, 15	8, 12
Γ_7	0, 18	6, 12	4, 8, 10, 14	2, 6, 8, 10, 12, 16	4, 6, 8, 10, 12, 14	5, 7, 11, 13	1, 7, 11, 17	3, 5, 7, 9^2, 11, 13, 15	8, 12
Γ_8	0, 4, 6^2, 8^4, 10^4, 12^2, 14, 18	2, 4^2, 6^3 8^2, 10^2, 12^3, 14^2, 16	4^3, 6^5, 8^8, 10^8, 12^5, 14^3	2^2, 4^3, 6^8, 8^{11}, 10^{11}, 12^8, 14^3, 16^2	2, 4^5, 6^8, 8^{10}, 10^{10}, 12^8, 14^5, 16	3, 5^4, 7^7, 9^8, 11^7, 13^4, 15	3, 5^4, 7^7, 9^8, 11^7, 13^4, 15	1, 3^4, 5^8, 7^{12}, 9^{14}, 11^{12}, 13^8, 15^4, 17	4^2, 6, 8

TABLE VII. Generating functions for tensors based on odd IR's of the double icosahedral group.

Γ_m \ Γ_r	Γ_1	Γ_2	Γ_3	Γ_4	Γ_5	Γ_6	Γ_7	Γ_8	Γ_9	Denom.
Γ_6	0, 30	2, 10, 12, 18, 20, 28	6, 10, 14, 16, 20, 24	6, 8, 12, 14, 16, 18, 22, 24	4, 8, 10, 12, 14, 16, 18, 20, 22, 26	1, 11, 19, 29	7, 13, 17, 23	3, 9, 11, 13 17, 19, 21, 27	5, 7, 9, 11, 13, 15^2, 17, 19, 21, 23, 25	12, 20
Γ_7	0, 30	6, 10, 14, 16, 20, 24	2, 10, 12, 18, 20, 28	6, 8, 12, 14, 16, 18, 22, 24	4, 8, 10, 12, 14, 16, 18, 20, 22, 26	7, 13, 17, 23	1, 11, 19, 29	3, 9, 11, 13, 17, 19, 21, 27	5, 7, 9, 11, 13, 15^2, 17, 19, 21, 23, 25	12, 20
Γ_8	0, 8^2, 10^2, 12^2, 20	2, 4, 6^3, 8^4, 10^6, 12^4, 14^3, 16, 18	2, 4, 6^3, 8^4, 10^6, 12^4, 14^3, 16, 18	2, 4^3, 6^5, 8^5, 10^4, 12^5, 14^5, 16^3, 18	4^3, 6^5, 8^8, 10^8, 12^8, 14^5, 16^3,	5, 7^3, 9^4, 11^4, 13^3, 15	5, 7^3, 9^4, 11^4, 13^3, 15	1, 3^2, 5^2, 7^4, 9^7, 11^7, 13^4, 15^2, 17^2, 19	3^2, 5^6, 7^8, 9^8, 11^8, 13^8, 15^6, 17^2	4^2, 6, 10
Γ_9	0, 4, 6^5, 8^{17}, 10^{22}, 12^{33}, 14^{34}, 16^{33}, 18^{22}, 20^{17}, 25^5, 24, 28	2^2, 4^5, 6^{20}, 8^{42}, 10^{74}, 12^{93}, 14^{104}, 16^{93}, 18^{74}, 20^{42}, 22^{20}, 24^5, 26^2	2^2, 4^5, 6^{20}, 8^{42}, 10^{74}, 12^{93}, 14^{104}, 16^{93}, 18^{74}, 20^{42}, 22^{20}, 24^5, 26^2	2, 4^8, 6^{28}, 8^{59}, 10^{93}, 12^{125}, 14^{140}, 16^{125}, 18^{93}, 20^{59}, 22^{28}, 24^8, 26	2, 4^{12}, 6^{32}, 8^{73}, 10^{119}, 12^{159}, 14^{168}, 16^{159}, 18^{119}, 20^{73}, 22^{32}, 24^{12}, 26	3, 5^8, 7^{23}, 9^{39}, 11^{54}, 13^{67}, 15^{67}, 17^{54}, 19^{39}, 21^{23}, 23^8, 25	3, 5^8, 7^{23}, 9^{39}, 11^{54}, 13^{67}, 15^{67}, 17^{54}, 19^{39}, 21^{23}, 23^8, 25	3^4, 5^{16}, 7^{40}, 9^{78}, 11^{114}, 13^{132}, 15^{132}, 17^{114}, 19^{78}, 21^{40}, 23^{16}, 25^4	1, 3^6, 5^{23}, 7^{60}, 9^{114}, 11^{169}, 13^{203}, 15^{203}, 17^{169}, 19^{114}, 21^{60}, 23^{23}, 25^6, 27	4^3, 6^2, 10

TABLE VIII. Generating elements for odd representations of ${}^{(d)}D_n$, ${}^{(d)}T$, and ${}^{(d)}O$ of dimension greater than one.

Group	Representation	Representation generating matrices
${}^{(d)}D_n$	Γ_r $r=5,7,\cdots$	$\begin{pmatrix}\exp\{\pi i(r-4)/n\} & 0\\ 0 & \exp\{-\pi i(r-4)/n\}\end{pmatrix}\begin{pmatrix}0 & i\\ i & 0\end{pmatrix}$
${}^{(d)}T$	Γ_5	$\frac{(1+i)}{2}\begin{pmatrix}-i & i\\ 1 & 1\end{pmatrix}$ $\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$
	Γ_6	$\frac{\omega(1+i)}{2}\begin{pmatrix}-i & i\\ 1 & 1\end{pmatrix}$ $\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$
	Γ_7	$\frac{\omega^2(1+i)}{2}\begin{pmatrix}-i & i\\ 1 & 1\end{pmatrix}$ $\begin{pmatrix}0 & -i\\ -i & 0\end{pmatrix}$
${}^{(d)}O$	Γ_6	$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & i\\ i & 1\end{pmatrix}$ $\frac{1+i}{2}\begin{pmatrix}-i & -1\\ -i & 1\end{pmatrix}$
	Γ_7	$\frac{-1}{\sqrt{2}}\begin{pmatrix}1 & i\\ i & 1\end{pmatrix}$ $\frac{1+i}{2}\begin{pmatrix}-i & -1\\ -i & 1\end{pmatrix}$
	Γ_8	$\frac{1}{\sqrt{8}}\begin{pmatrix}1 & \sqrt{3}i & -\sqrt{3} & -i\\ \sqrt{3}i & -1 & i & -\sqrt{3}\\ -\sqrt{3} & i & -1 & \sqrt{3}i\\ -i & -\sqrt{3}i & \sqrt{3}i & 1\end{pmatrix}$
		$\frac{1+i}{4}\begin{pmatrix}-1 & \sqrt{3}i & \sqrt{3} & -i\\ -\sqrt{3} & i & -1 & \sqrt{3}i\\ -\sqrt{3} & -i & -1 & -\sqrt{3}i\\ -1 & -\sqrt{3}i & \sqrt{3} & i\end{pmatrix}$

$$E^{(8)}_{3,5}=\alpha^8+4\sqrt{3}\,i\alpha^6\beta^2-10\alpha^4\beta^4+4\sqrt{3}\,i\alpha^2\beta^6+\beta^8,$$

$$E^{(2)}_{4,5}=\begin{bmatrix}\alpha^2-\beta^2\\ -i(\alpha^2+\beta^2)\\ 2\alpha\beta\end{bmatrix},\quad E^{(4)}_{4,5}=\begin{bmatrix}2\alpha\beta(\alpha^2+\beta^2)\\ 2i\alpha\beta(\alpha^2-\beta^2)\\ \alpha^4-\beta^4\end{bmatrix},$$

$$E^{(6)a}_{4,5}=\begin{bmatrix}(\alpha^2-\beta^2)^3\\ i(\alpha^2+\beta^2)^3\\ 8\alpha^3\beta^3\end{bmatrix},\quad E^{(6)b}_{4,5}=\begin{bmatrix}4\alpha^2\beta^2(\alpha^2-\beta^2)\\ -i(\alpha^2-\beta^2)(\alpha^4-\beta^4)\\ -2\alpha\beta(\alpha^2+\beta^2)^2\end{bmatrix},$$

$$E^{(8)}_{4,5}=\begin{bmatrix}8\alpha^3\beta^3(\alpha^2+\beta^2)\\ 2i\alpha\beta(\alpha^2-\beta^2)^3\\ -(\alpha^2+\beta^2)^2(\alpha^4-\beta^4)\end{bmatrix},\quad E^{(10)}_{4,5}=\begin{bmatrix}16\alpha^4\beta^4(\alpha^2-\beta^2)\\ -i(\alpha^2-\beta^2)^3(\alpha^4-\beta^4)\\ 2\alpha\beta(\alpha^2+\beta^2)^4\end{bmatrix}$$

$$E^{(1)}_{5,5}=\begin{bmatrix}\alpha\\ \\ \beta\end{bmatrix},\quad E^{(5)}_{5,5}=\begin{bmatrix}\alpha^5-5\alpha\beta^4\\ \\ \beta^5-5\alpha^4\beta\end{bmatrix},$$

$$E^{(7)}_{5,5}=\begin{bmatrix}\beta^7+7\alpha^4\beta^3\\ -\alpha^7-7\alpha^3\beta^4\end{bmatrix},\quad E^{(11)}_{5,5}=\begin{bmatrix}\beta^{11}-22\alpha^4\beta^7-11\alpha^8\beta^3\\ -\alpha^{11}+22\alpha^7\beta^4+11\alpha^3\beta^8\end{bmatrix},$$

$$E^{(3)}_{6,5}=\begin{bmatrix}\beta^3+\sqrt{3}\,i\alpha^2\beta\\ -\alpha^3-\sqrt{3}\,i\alpha\beta^2\end{bmatrix},\quad E^{(5)}_{6,5}=\begin{bmatrix}\alpha^5+2\sqrt{3}\,i\alpha^3\beta^2+\alpha\beta^4\\ \beta^5+2\sqrt{3}\,i\alpha^2\beta^3+\alpha^4\beta\end{bmatrix},$$

$$E^{(7)}_{6,5}=\begin{bmatrix}\beta^7-3\sqrt{3}\,i\alpha^2\beta^5-5\alpha^4\beta^3-\sqrt{3}\,i\alpha^6\beta\\ -\alpha^7+3\sqrt{3}\,i\alpha^5\beta^2+5\alpha^3\beta^4+\sqrt{3}\,i\alpha\beta^6\end{bmatrix},$$

$$E^{(9)}_{6,5}=\begin{bmatrix}\alpha^9-4\sqrt{3}\,i\alpha^7\beta^2-10\alpha^5\beta^4-4\sqrt{3}\,i\alpha^3\beta^6+\alpha\beta^8\\ \beta^9-4\sqrt{3}\,i\alpha^2\beta^7-10\alpha^4\beta^5-4\sqrt{3}\,i\alpha^6\beta^3+\alpha^8\beta\end{bmatrix},$$

$$E^{(3)}_{7,5}=\begin{bmatrix}\beta^3-\sqrt{3}\,i\alpha^2\beta\\ -\alpha^3+\sqrt{3}\,i\alpha\beta^2\end{bmatrix},\quad E^{(5)}_{7,5}=\begin{bmatrix}\alpha^5-2\sqrt{3}\,i\alpha^3\beta^2+\alpha\beta^4\\ \beta^5-2\sqrt{3}\,i\alpha^2\beta^3+\alpha^4\beta\end{bmatrix},$$

$$E^{(7)}_{7,5}=\begin{bmatrix}\beta^7+3\sqrt{3}\,i\alpha^2\beta^5-5\alpha^4\beta^3+\sqrt{3}\,i\alpha^6\beta\\ -\alpha^7-3\sqrt{3}\,i\alpha^5\beta^2+5\alpha^3\beta^4-\sqrt{3}\,i\alpha\beta^6\end{bmatrix},$$

$$E^{(9)}_{7,5}=\begin{bmatrix}\alpha^9+4\sqrt{3}\,i\alpha^7\beta^2-10\alpha^5\beta^4+4\sqrt{3}\,i\alpha^3\beta^6+\alpha\beta^8\\ \beta^9+4\sqrt{3}\,i\alpha^2\beta^7-10\alpha^4\beta^5+4\sqrt{3}\,i\alpha^6\beta^3+\alpha^8\beta\end{bmatrix}. \tag{16}$$

The IR's Γ_6 and Γ_7 are mutually conjugate. The elementary tensors based on them are

$$E^{(8)}_{2,6}=E^{(8)}_{3,5},\qquad E^{(8)}_{3,7}=E^{(8)}_{2,5},$$

$$E^{(4)}_{3,6}=E^{(4)}_{2,5},\qquad E^{(4)}_{2,7}=E^{(4)}_{3,5},$$

$$E^{(2)}_{4,6}=\begin{bmatrix}\alpha^2-\beta^2\\ -i\omega^2(\alpha^2+\beta^2)\\ 2\alpha\beta\end{bmatrix},\quad E^{(2)}_{4,7}=\begin{bmatrix}\alpha^2-\beta^2\\ i\omega(\alpha^2+\beta^2)\\ 2\alpha\beta\end{bmatrix},$$

$$E^{(4)}_{4,6}=\begin{bmatrix}2\omega^2(\alpha^3\beta+\alpha\beta^3)\\ 2i(\alpha^3\beta-\alpha\beta^3)\\ \omega(\alpha^4-\beta^4)\end{bmatrix},\quad E^{(4)}_{4,7}=\begin{bmatrix}2\omega(\alpha^3\beta+\alpha\beta^3)\\ -2i(\alpha^3\beta-\alpha\beta^3)\\ \omega^2(\alpha^4-\beta^4)\end{bmatrix},$$

$$E^{(6)}_{4,6}=\begin{bmatrix}(\alpha^2-\beta^2)^3\\ i(\alpha^2+\beta^2)^3\\ 8\alpha^3\beta^3\end{bmatrix},\quad E^{(6)}_{4,7}=\begin{bmatrix}(\alpha^2-\beta^2)^3\\ -i(\alpha^2+\beta^2)^3\\ 8\alpha^3\beta^3\end{bmatrix},$$

$$E^{(5)}_{5,6}=E^{(5)}_{6,5},\quad E^{(5)}_{5,7}=E^{(5)}_{7,5},$$

$$E^{(7)}_{5,6}=E^{(7)}_{7,5},\quad E^{(7)}_{5,7}=E^{(7)}_{6,5},$$

$$E^{(1)}_{6,6}=E^{(1)}_{7,7}=E^{(1)}_{5,5},$$

$$E^{(3)}_{6,6}=E^{(3)}_{6,5},\quad E^{(3)}_{7,7}=E^{(3)}_{7,5},$$

$$E^{(3)}_{7,6}=E^{(3)}_{7,5},\quad E^{(3)}_{6,7}=E^{(3)}_{6,5},$$

$$E^{(5)}_{7,6}=E^{(5)}_{6,7}=E^{(5)}_{5,5}. \tag{17}$$

An equation like $E^{(7)}_{5,6}=E^{(7)}_{7,5}$ in (21) is meant to imply only that the dependence of the components on $\alpha,\beta,\cdots$ is the same on both sides of the equation; the variables, however, have quite different meanings on the two sides.

${}^{(d)}O$ tensors

The degrees of the scalars and tensors based on the odd IR's, Γ_6, Γ_7, Γ_8, of ${}^{(d)}O$ may be read from Table VII. For reasons of space we give here only those based on the conjugate IR's Γ_6 and Γ_7.

The elementary scalars are

$$I^{(8)}_6=I^{(8)}_7=\alpha^8+14\alpha^4\beta^4+\beta^8,$$

$$I^{(12)}_6=I^{(12)}_7=\alpha^{10}\beta^2-2\alpha^6\beta^6+\alpha^2\beta^{10}. \tag{18}$$

$$E^{(18)}_{1,6}=E^{(18)}_{1,7}=\alpha^{17}\beta-34\alpha^{13}\beta^5+34\alpha^5\beta^{13}-\alpha\beta^{17}.$$

The other elementary tensors are as follows:

$$E^{(6)}_{2,6}=E^{(6)}_{2,7}=\alpha^5\beta-\alpha\beta^5,\qquad E^{(12)}_{2,6}=E^{(12)}_{2,7}=\alpha^{12}-33\alpha^8\beta^4-33\alpha^4\beta^8+\beta^{12},$$

$$E^{(4)}_{3,6}=E^{(4)}_{3,7}=\begin{bmatrix}\sqrt{3}\,(\alpha^4+6\alpha^2\beta^2+\beta^4)\\ -3(\alpha^2-\beta^2)^2\end{bmatrix}.\qquad E^{(8)}_{3,6}=E^{(8)}_{3,7}=\begin{bmatrix}\sqrt{3}\,(\alpha^8+4\alpha^6\beta^2-10\alpha^4\beta^4+4\alpha^2\beta^6+\beta^8)\\ \alpha^8-12\alpha^6\beta^2-10\alpha^4\beta^4-12\alpha^2\beta^6+\beta^8\end{bmatrix},$$

$$E^{(10)}_{3,6}=E^{(10)}_{3,7}=(\alpha^5\beta-\alpha\beta^5)\begin{bmatrix}(\alpha^2-\beta^2)^2\\ \sqrt{3}(\alpha^4+6\alpha^2\beta^2+\beta^4)\end{bmatrix},$$

$$E^{(14)}_{3,6}=E^{(14)}_{3,7}=(\alpha^5\beta-\alpha\beta^5)\begin{bmatrix}\alpha^8-12\alpha^6\beta^2-10\alpha^4\beta^4-12\alpha^2\beta^6+\beta^8\\ \sqrt{3}\,(\alpha^8+4\alpha^6\beta^2-10\alpha^4\beta^4+4\alpha^2\beta^6+\beta^8)\end{bmatrix},$$

$$E^{(2)}_{4,6}=E^{(2)*}_{4,7}=\begin{bmatrix}\alpha^2-\beta^2\\ -i(\alpha^2+\beta^2)\\ 2\alpha\beta\end{bmatrix},\qquad E^{(6)}_{4,6}=E^{(6)*}_{4,7}=\begin{bmatrix}\alpha^6-3\alpha^4\beta^2+3\alpha^2\beta^4-\beta^6\\ i(\alpha^6+3\alpha^4\beta^2+3\alpha^2\beta^4+\beta^6)\\ 8\alpha^3\beta^3\end{bmatrix},$$

$$E^{(8)}_{4,6}=E^{(8)*}_{4,7}=\begin{bmatrix}i(\alpha^7\beta+7\alpha^5\beta^3+7\alpha^3\beta^5+\alpha\beta^7)\\ -\alpha^7\beta+7\alpha^5\beta^3-7\alpha^3\beta^5+\alpha\beta^7\\ -\alpha^8+\beta^8\end{bmatrix},$$

$$E^{(10)}_{4,6}=E^{(10)*}_{4,7}=\begin{bmatrix}\alpha^{10}-5\alpha^8\beta^2+10\alpha^6\beta^4-10\alpha^4\beta^6+5\alpha^2\beta^8-\beta^{10}\\ -i(\alpha^{10}+5\alpha^8\beta^2+10\alpha^6\beta^4+10\alpha^4\beta^6+5\alpha^2\beta^8+\beta^{10})\\ 32\alpha^5\beta^5\end{bmatrix},$$

$$E^{(12)}_{4,6}=E^{(12)*}_{4,7}=\begin{bmatrix}\alpha^{11}\beta+5\alpha^9\beta^3-6\alpha^7\beta^5-6\alpha^5\beta^7+5\alpha^3\beta^9+\alpha\beta^{11}\\ -i(\alpha^{11}\beta-5\alpha^9\beta^3-6\alpha^7\beta^5+6\alpha^5\beta^7+5\alpha^3\beta^9-\alpha\beta^{11})\\ 4(-\alpha^{10}\beta^2+\alpha^2\beta^{10})\end{bmatrix},$$

$$E^{(16)}_{4,6}=E^{(16)*}_{4,7}=\begin{bmatrix}\alpha^{15}\beta+7\alpha^{13}\beta^3+21\alpha^{11}\beta^5+99\alpha^9\beta^7+99\alpha^7\beta^9+21\alpha^5\beta^{11}+7\alpha^3\beta^{13}+\alpha\beta^{15}\\ i(\alpha^{15}\beta-7\alpha^{13}\beta^3+21\alpha^{11}\beta^5-99\alpha^9\beta^7+99\alpha^7\beta^9-21\alpha^5\beta^{11}+7\alpha^3\beta^{13}-\alpha\beta^{15})\\ -\alpha^{16}-14\alpha^{12}\beta^4+14\alpha^4\beta^{12}+\beta^{16}\end{bmatrix},$$

$$E^{(4)}_{5,6}=E^{(4)*}_{5,7}=\begin{bmatrix}2(\alpha^3\beta+\alpha\beta^3)\\ \alpha^4-\beta^4\\ 2i(\alpha^3\beta-\alpha\beta^3)\end{bmatrix},\qquad E^{(6)}_{5,6}=\begin{bmatrix}\alpha^6+5\alpha^4\beta^2-5\alpha^2\beta^4-\beta^6\\ -4(\alpha^5\beta+\alpha\beta^5)\\ -i(\alpha^6-5\alpha^4\beta^2-5\alpha^2\beta^4+\beta^6)\end{bmatrix}\qquad E^{(8)}_{4,6}=E^{(8)*}_{4,7}=\begin{bmatrix}\alpha^7\beta-\alpha^5\beta^3-\alpha^3\beta^5+\alpha\beta^7\\ 2(\alpha^6\beta^2-\alpha^2\beta^6)\\ i(-\alpha^7\beta-\alpha^5\beta^3+\alpha^3\beta^5+\alpha\beta^7)\end{bmatrix},$$

$$E^{(10)}_{5,6}=E^{(10)*}_{5,7}=\begin{bmatrix}-\alpha^{10}-3\alpha^8\beta^2+14\alpha^6\beta^4-14\alpha^4\beta^6+3\alpha^2\beta^8+\beta^{10}\\ 16(\alpha^7\beta^3+\alpha^3\beta^7)\\ i(-\alpha^{10}+3\alpha^8\beta^2+14\alpha^6\beta^4+14\alpha^4\beta^6+3\alpha^2\beta^8-\beta^{10})\end{bmatrix},$$

$$E^{(12)}_{5,6}=E^{(12)*}_{5,7}=\begin{bmatrix}\alpha^{11}\beta-3\alpha^9\beta^3+2\alpha^7\beta^5+2\alpha^5\beta^7-3\alpha^3\beta^9+\alpha\beta^{11}\\ 8(\alpha^8\beta^4-\alpha^4\beta^8)\\ i(\alpha^{11}\beta+3\alpha^9\beta^3+2\alpha^7\beta^5-2\alpha^5\beta^7-3\alpha^3\beta^9-\alpha\beta^{11})\end{bmatrix},$$

$$E^{(14)}_{5,6}=E^{(14)*}_{5,7}=\begin{bmatrix}\alpha^{14}+5\alpha^{12}\beta^2+9\alpha^{10}\beta^4+69\alpha^8\beta^6-69\alpha^6\beta^8-9\alpha^4\beta^{10}-5\alpha^2\beta^{12}-\beta^{14}\\ -4(\alpha^{13}\beta+15\alpha^9\beta^5+15\alpha^5\beta^9+\alpha\beta^{13})\\ -i(\alpha^{14}-5\alpha^{12}\beta^2+9\alpha^{10}\beta^4-69\alpha^8\beta^6-69\alpha^6\beta^8+9\alpha^4\beta^{10}-5\alpha^2\beta^{12}+\beta^{14})\end{bmatrix}$$

$$E^{(1)}_{6,6}=E^{(1)}_{7,7}=\begin{bmatrix}\alpha\\ \beta\end{bmatrix},\qquad E^{(7)}_{6,6}=E^{(7)}_{7,7}=\begin{bmatrix}\beta^7+7\alpha^4\beta^3\\ \alpha^7+7\alpha^3\beta^4\end{bmatrix},$$

$$E^{(11)}_{6,6}=E^{(11)}_{7,7}=\begin{bmatrix}\alpha^{10}\beta-6\alpha^6\beta^5+5\alpha^2\beta^9\\ \alpha\beta^{10}-6\alpha^5\beta^6+5\alpha^9\beta^2\end{bmatrix},$$

$$E^{(17)}_{6,6}=E^{(17)}_{7,7}=\begin{bmatrix}\alpha^{17}+28\alpha^{13}\beta^4+198\alpha^9\beta^8+28\alpha^5\beta^{12}+\alpha\beta^{16}\\ \beta^{17}+28\alpha^4\beta^{13}+198\alpha^8\beta^9+28\alpha^{12}\beta^5+\alpha^{16}\beta\end{bmatrix},$$

$$E^{(5)}_{7,6}=E^{(5)}_{6,7}=\begin{bmatrix}\alpha^5-5\alpha\beta^4\\ \beta^5-5\alpha^4\beta\end{bmatrix},\qquad E^{(7)}_{7,6}=E^{(7)}_{6,7}=\begin{bmatrix}\alpha^6\beta-\alpha^2\beta^5\\ \alpha\beta^6-\alpha^5\beta^2\end{bmatrix},$$

$$E^{(11)}_{7,6}=E^{(11)}_{6,7}=\begin{bmatrix}\beta^{11}-22\alpha^4\beta^7-11\alpha^8\beta^3\\ \alpha^{11}-22\alpha^7\beta^4-11\alpha^3\beta^8\end{bmatrix},\qquad E^{(13)}_{7,6}=E^{(13)}_{6,7}=\begin{bmatrix}\alpha^{13}-26\alpha^9\beta^4-39\alpha^5\beta^8\\ \beta^{13}-26\alpha^4\beta^9-39\alpha^8\beta^5\end{bmatrix},$$

$$E^{(3)}_{8,6}=E^{(3)}_{8,7}=\begin{bmatrix}\alpha^3\\ -\sqrt{3}\,\alpha^2\beta\\ -\sqrt{3}\,\alpha\beta^2\\ \beta^3\end{bmatrix},\quad E^{(5)}_{8,6}=E^{(5)}_{8,7}=\begin{bmatrix}\alpha^4\beta+\beta^5\\ 2\sqrt{3}\,\alpha^3\beta^2\\ -2\sqrt{3}\,\alpha^2\beta^3\\ -\alpha\beta^4-\alpha^5\end{bmatrix},\quad E^{(7)}_{8,6}=E^{(7)}_{8,7}=\begin{bmatrix}\sqrt{3}\,(3\alpha^5\beta^2+\alpha\beta^6)\\ 5\alpha^4\beta^3-\beta^7\\ 5\alpha^3\beta^4-\alpha^7\\ \sqrt{3}\,(3\alpha^2\beta^5+\alpha^6\beta)\end{bmatrix},$$

$$E^{(9)a}_{8,6}=E^{(9)a}_{8,7}=\begin{bmatrix}-2\sqrt{3}(3\alpha^6\beta^3+\alpha^2\beta^7)\\ \alpha^9-8\alpha^5\beta^4-\alpha\beta^8\\ -\beta+8\alpha^4\beta^5+\alpha^8\beta\\ -2\sqrt{3}(3\alpha^3\beta^6+\alpha^7\beta^2)\end{bmatrix},\qquad E^{(9)b}_{8,6}=E^{(9)b}_{8,7}=\begin{bmatrix}4\sqrt{3}(\alpha^6\beta^3+\alpha^2\beta^7)\\ \alpha^9-10\alpha^5\beta^4+\alpha\beta^8\\ -\beta^9+10\alpha^4\beta^5-\alpha^8\beta\\ -4\sqrt{3}(\alpha^3\beta^6+\alpha^7\beta^2)\end{bmatrix},$$

$$E^{(11)}_{8,6}=E^{(11)}_{8,7}=\begin{bmatrix}\alpha^{11}+8\alpha^7\beta^4+7\alpha^3\beta^8\\ -2\sqrt{3}\,(7\alpha^6\beta^5+\alpha^2\beta^9)\\ -2\sqrt{3}\,(7\alpha^5\beta^6+\alpha^9\beta^2)\\ \beta^{11}+8\alpha^4\beta^7+7\alpha^8\beta^3\end{bmatrix},\qquad E^{(13)}_{8,6}=E^{(13)}_{8,7}=\begin{bmatrix}\alpha^{12}\beta-6\alpha^8\beta^5+5\alpha^4\beta^9\\ \sqrt{3}\,(\alpha^{11}\beta^2+2\alpha^7\beta^6-3\alpha^3\beta^{10})\\ -\sqrt{3}\,(\alpha^2\beta^{11}+2\alpha^6\beta^7-3\alpha^{10}\beta^3)\\ -\alpha\beta^{12}+6\alpha^5\beta^8-5\alpha^9\beta^4\end{bmatrix},$$

$$E^{(15)}_{8,6}=E^{(15)}_{8,7}=\begin{bmatrix}8\sqrt{3}\,(\alpha^{13}\beta^2+2\alpha^9\beta^6-12\alpha^5\beta^{10}+\alpha\beta^{14})\\ \beta^{15}+43\alpha^2\beta^{13}-159\alpha^4\beta^{11}+51\alpha^8\beta^7\\ \alpha^{15}+43\alpha^{13}\beta^2-159\alpha^{11}\beta^4+51\alpha^7\beta^8\\ 8\sqrt{3}\,(\alpha^2\beta^{13}+2\alpha^6\beta^9-12\alpha^{10}\beta^5+\alpha^{14}\beta)\end{bmatrix}. \tag{19}$$

4. DOUBLE GROUP BASES OF SU(2)

It is desirable to construct basis states of SU(2), reduced according to its subgroup ${}^{(d)}G$, where ${}^{(d)}G$ is any double point group. Since the subgroup representation and component labels take only a finite number of values, they do not "count" as labels in Racah's sense. There is thus one missing label.

As usual there are two complementary approaches to the labeling problem. One is to construct a missing label operator. It should be a ${}^{(d)}G$ scalar which is a polynomial in the SU(2) generators. Since there is one missing label, there should be two functionally independent missing label operators in each case.[4]

The missing label operators may be read from the results of Ref. 1 for the groups ${}^{(d)}C_n$, ${}^{(d)}D_n$, ${}^{(d)}T$, or ${}^{(d)}O$. They are just the C_n, D_n, T, or O scalars (a G scalar is also a ${}^{(d)}G$ scalar) formed from L_x, L_y, L_z which, of course, transform like x, y, z; in each case the quadratic scalar L^2 should be disregarded. Thus we find the following missing label operators:

$$\begin{aligned}&{}^{(d)}C_n \text{ or } C_n\text{: } L_z,\ L_+^n+L_-^n,\\ &{}^{(d)}D_n \text{ or } D_n\text{: } L_z^2,\ L_+^n+L_-^n,\\ &{}^{(d)}T \text{ or } T\text{: } L_xL_yL_z,\ L_x^4+L_y^4+L_z^4,\\ &{}^{(d)}O \text{ or } O\text{: } L_xL_yL_z,\ L_x^4+L_y^4+L_z^4.\end{aligned} \tag{20}$$

It is understood that the operator $L_xL_yL_z$ should be symmetrized with respect to the ordering of the factors. For ${}^{(d)}I$ or I, according to the generating function $B_{1,2}(\lambda)$, the two missing label operators are of degrees 6 and 10 in L_x, L_y, L_z. Another, of degree 15, is the square root of a polynomial in the lower degree scalars and L^2. For a more detailed discussion of the labeling operators see Bickerstaff and Wybourne.[5]

We now turn to a second approach to ${}^{(d)}G$ polynomial basis states for SU(2). Such states are already constructed in Sec. 3. They are just the components of the polynomial tensors described by the generating function $B_{r,s}(\lambda)$, where Γ_s is the representation of ${}^{(d)}G$ contained in the $j=\frac{1}{2}$ (spinor) representation of SU(2).

The $j=\frac{1}{2}$ IR of SU(2) contains the following representations Γ_s of the double point groups:

$$\begin{aligned}\Gamma_s&=\Gamma_2\oplus\Gamma_{2n} \text{ for } {}^{(d)}C_n,\\ &=\Gamma_5 \text{ for } {}^{(d)}D_n,\\ &=\Gamma_5 \text{ for } {}^{(d)}T,\\ &=\Gamma_6 \text{ for } {}^{(d)}O,\\ &=\Gamma_6 \text{ for } {}^{(d)}I.\end{aligned} \tag{21}$$

Except for ${}^{(d)}C_n$, Γ_s is irreducible, so the polynomials are already given in Sec. 3 for ${}^{(d)}D_n$, ${}^{(d)}T$, and ${}^{(d)}O$. For ${}^{(d)}C_n$, the Wigner monomial $\alpha^a\beta^b$ is already an irreducible ${}^{(d)}C_n$ tensor, transforming by the IR Γ_r, where $r=(a-b)_{\mathrm{mod}\,2n}+2$.

As an example let us discuss ${}^{(d)}T$ in more detail. The SU(2) basis states are

$$(E^{(p)}_{r,5})_t(\alpha^5\beta-\alpha\beta^5)^a(\alpha^8+14\alpha^4\beta^4+\beta^8)^b, \tag{22}$$

where $(E^{(p)}_{r,5})_t$ denotes the t component of the tensor $E^{(p)}_{r,5}$. The SU(2) IR label j is one-half the degree of the polynomial:

$$j=\tfrac{1}{2}(p+6a+8b). \tag{23}$$

When j and p are specified, a and b are not independent

and one of them may be regarded as the missing label. The basis states (22) are not orthonormal in general, but have the advantage of being analytic. The even states (j integral) constitute a convenient basis for the SO(3) $\supset T$ scheme. It is no accident that the generating function $B_{\Gamma_r,5}(\lambda)$, with Γ_r even, is equal to $(1-\lambda^2)B_{\Gamma_r,1}(\lambda^2)$.

The states described here lend themselves to the calculation of generator and finite rotation matrix elements as well as reduced Wigner (or Clebsch–Gordan) coefficients in an $SU(2)\supset {}^{(d)}G$ [or $SO(3)\supset G$] basis.

5. CONCLUDING REMARKS

The methods employed in this paper and in I can be applied to construct polynomial tensors of arbitrary degree in the components of any finite group tensor.

The construction of $SU(2)\supset {}^{(d)}G$ basis states effected here for a double point group ${}^{(d)}G$ can be extended to find analytic finite subgroup bases for any continuous group. The starting point is a generating function for the weights contained in any IR of the continous group.[6] Such a generating function is converted to a generating function for finite subgroup IR's by the methods of I and this article and leads to the determination of an integrity basis for subgroup states. This opens the possibility of constructing the Racah algebra (generator matrix elements, coupling coefficients etc.) for the continuous group in a finite subgroup basis.

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Higher order modified potentials for the effective phase integral approximation[a)]

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Higher order modified potentials for the effective phase integral approximation are derived from first principles. Application is made to computing eigenvalues for a nearly free wavefunction in a lattice potential.

I. INTRODUCTION

Recently the phase integral approximation has been modified by incorporating an energy-dependent modified (heretofore effective) potential that is consistent to first order in potential.[1] This modification extends the domain of applicability of the phase integral approximation to longer wavelengths. When applied to the geometric theory of wave propagation, this modification generates a wavelength dependence in the consequent effective index of refraction which may be used to determine the stationary ray paths.[2] Herein from first principles, we develop and investigate higher order terms of the modified potential. While we use a lattice potential for continuity with first order results[1] where band implications were discussed, herein we concentrate on higher order techniques and not on band aspects, and without loss of generality we use mostly energy quantizations that are centered in the allowed energy bands.

In Sec. II we develop the higher order terms of the modified potential for a general potential, make application to the lattice potential appearing in Mathieu's equation, and illustrate numerical accuracy with examples. Section III presents a comparison to Fröman and Fröman's expansion.

II. EXPANSION OF THE MODIFIED POTENTIAL

Let us express the time independent Schrödinger equation in one dimension, x, as

$$\frac{d^2\psi(x)}{dx^2}+\frac{2\mu}{\hbar^2}\left[E-\lambda V(x)\right]\psi(x)=0, \tag{1}$$

where as usual ψ is the wavefunction, μ is mass, $\hbar=1.0545887\times10^{-27}$ erg sec and E is energy, but where an explicit expansion parameter λ is associated with the potential V. The solution to Eq. (1) may be found by substituting

$$\psi_{\pm}(x)=\left\{\frac{2\mu}{\hbar^2}\left[E-\lambda W(E,\lambda,x)\right]\right\}^{-1/4}\times\exp\left(\pm i\int^x\left\{\frac{2\mu}{\hbar^2}\left[E-\lambda W(E,\lambda,x')\right]\right\}^{1/2}dx'\right),$$

where W is our new variable. W may be identified as the energy-dependent modified potential (previously identified as effective potential[1]). This leads to the nonlinear differential equation for $W(E,\lambda,x)$,

$$W=V-\frac{\hbar^2}{8\mu}\frac{W''}{E-\lambda W}-\frac{5\hbar^2}{32\mu}\frac{\lambda(W')^2}{(E-\lambda W)^2}. \tag{2}$$

For $|\lambda W|<E$, Eq. (2) may be expanded as

$$W=V-\frac{\hbar^2}{8\mu}\frac{W''}{E}\sum_{n=0}^{\infty}\left(\frac{\lambda W}{E}\right)^n-\frac{5\hbar^2}{32\mu}\lambda\left(\frac{W'}{E}\right)^2\sum_{n=0}^{\infty}(1+n)\left(\frac{\lambda W}{E}\right)^n. \tag{3}$$

Let us also expand W in a power series of λ as

$$W=W_0+\lambda W_1+\lambda^2W_2\cdots$$

and substitute this into Eq. (3). Upon equating all coefficients of like powers of λ, we have that[3]

$$W_0''+\frac{8\mu}{\hbar^2}EW_0=\frac{8\mu}{\hbar^2}EV, \tag{4a}$$

$$W_1''+\frac{8\mu}{\hbar^2}EW_1=-\frac{W_0W_0''}{E}-\frac{5}{4}\frac{(W_0')^2}{E}, \tag{4b}$$

$$W_2''+\frac{8\mu}{\hbar^2}EW_2=\frac{-W_1''W_0}{E}-\frac{W_1W_0''}{E}-\frac{5}{2}\frac{W_1'W_0'}{E}-\frac{W_0^2W_0''}{E^2}-\frac{5}{2}\frac{W_0(W_0')^2}{E^2}, \tag{4c}$$

$$W_3''+\frac{8\mu}{\hbar^2}EW_3=-\frac{W_0W_2''}{E}-\frac{W_2W_0''}{E}-\frac{W_1W_1''}{E}-\frac{2W_0W_1W_0''}{E^2}-\frac{W_0^2W_1''}{E^2}-\frac{W_0^3W_0''}{E^3}-\frac{5}{2}\frac{W_2'W_0'}{E}-\frac{5}{4}\frac{(W_1')^2}{E}-\frac{5}{2}\frac{W_1(W_0')^2}{E^2}-5\frac{W_0W_0'W_1'}{E^2}-\frac{15}{4}\frac{W_0^2(W_0')^2}{E^3}, \tag{4d}$$

$$W_n''+\frac{8\mu}{\hbar^2}EW_n=f(W_{n-1},\ W_{n-2},\ \ldots,\ W_0,\ W_{n-1}',\ W_{n-2}',\ \ldots,\ W_0',\ W_{n-1}'',\ W_{n-2}'',\ \ldots,\ W_0''),\quad n=1,\ 2,\ 3,\ \ldots, \tag{4e}$$

where f is a driving function. Equation (4a), the first order equation, has been investigated previously.[1] It is noted that the left sides of Eqs. (4a)–(4d) as well as the general case, Eq. (4e), all have the simple form of the reduced wave equation with constant coefficients while the right sides represent inhomogeneous driving functions whose entire components may be established directly from preceding lower order results. Therefore, the first few higher order results are easily obtained while in principle all other finite higher order results may be calculated directly. However, the convergence of the expansion of the modified potential (over its

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TABLE I. Calculated eigenvalues, α's, of Mathieu's equation, $\psi''+(\alpha-2\gamma\cos 2x)\psi=0$ for selected γ and selected values of the characteristic exponent ν and for various truncations N of the expansion of the effective potential $W^{(N)}(\alpha,x)$.

Characteristic exponent, ν		0.3	3.5	4.5	5.5
γ		0.03	1.0	1.0	1.0
α	Rounded-off exact	0.08950555848	12.294632	20.27600336	30.26710156
α	$N=0$	0.09004898232	12.298481	20.27734259	30.26768419
α	$N=1$	0.08950548469	12.294749	20.27601384	30.26710329
α	$N=2$	0.08950607239	12.294803	20.27601766	30.26710398
α	$N=3$	0.08950555853	12.294659	20.27600363	30.26710157

x-domain) cannot be assured for arbitrary forms of the potential $V(x)$, and in general all orders of W_n will be energy dependent.

In the specific case of the lattice potential appearing in Mathieu's equation, i.e., $V(x)=2\gamma\cos 2x$ with $\lambda=1$, $(2\mu/\hbar^2)=1$, and the associated eigenvalue being given as $\alpha=E$, the expansion for the modified potential for the first four terms is given by

$$W_0=\frac{2\gamma\cos 2x}{1-\alpha^{-1}}, \tag{5a}$$

$$W_1=\frac{\gamma^2}{2(\alpha-1)^2}\left[-1+\frac{9\cos 4x}{1-4\alpha^{-1}}\right], \tag{5b}$$

$$W_2=\frac{\gamma^3}{(\alpha-1)^3}\left[\cos 2x+\frac{A\cos 6x}{1-9\alpha^{-1}}\right], \tag{5c}$$

$$W_3=\frac{\gamma^4}{(\alpha-1)^4}\left\{-1.5-\frac{6.75}{\alpha-4}-\frac{10.125}{(\alpha-4)^2}+\left[8\alpha+\frac{2.5A\alpha}{1-9\alpha^{-1}}-\frac{9}{\alpha-4}+\frac{31.5}{1-4\alpha^{-1}}\right]\frac{\cos 4x}{(\alpha-4)}+\left[9.5+\frac{17.5A}{\alpha-9}-\frac{81.625}{\alpha-4}+\frac{91.125}{(\alpha-4)^2}\right]\frac{\alpha\cos 8x}{\alpha-16}\right\}, \tag{5d}$$

where $A=\{[45/(\alpha-4)]+7\}$. As expected, W_n has singularities at $\alpha=m^2$, where $m=\pm n$ and usually also $m=\pm 1,\pm 2,\ldots,\pm n\mp 1$ which manifests the mth order band gaps for the eigenvalues. This manifestation of nth order Bragg reflection is innate for W_n.

For relatively free wavefunctions (i.e., $E\gg V$), the results of at least the first four terms of the expansion of the modified potential, Eqs. (4a)–(4d), are in general good. Let us illustrate by calculating some eigenvalues α for the lattice potential appearing in Mathieu's equation from the quantization of the effective action variable associated with the modified potential, that is,[1]

$$\int_0^{\pi}[\alpha-W(\alpha,\lambda,x)]^{1/2}\,dx=\nu\pi,\quad|\nu|\neq 1,2,3,\cdots, \tag{6}$$

where ν is the given characteristic exponent (Bloch wavenumber) which establishes the quantization, $\lambda=1$ and $(2\mu/\hbar^2)=1$. Let us define the partial sum of the power series expansion for $W(\alpha,\lambda,x)$ by N such that

$$W^{(N)}(\alpha,\lambda,x)=\sum_{n=0}^{N}\lambda^n W_n(\alpha,x). \tag{7}$$

Table I exhibits the computations of energy levels (i.e., eigenvalues) for various partial sums of order N of Eq. (7) for various lattice potentials that are sufficiently small to render nearly free electrons. While the calculations for $N=3$ show excellent numerical approximations to the tabulated values even for long (with respect to lattice spacing) wavelengths, $\nu=0.3$, where the WKB approximation fails,[1] the numerical improvement is not monotonic with N as the estimates for α with $N=2$ are all inferior to those for $N=1$. Also for $\nu=0.3$ and $\gamma=0.03$, the $N=0$ estimate for α is inferior to the plane wave limit (i.e., $\alpha=\nu^2$); nevertheless, it has already been shown[1] that for this case a more sophisticated estimate based upon the expected value of the Hamiltonian H, (i.e., $\alpha=\int\psi^\dagger H\psi dx/\int\psi^\dagger\psi dx$, where $\psi=(\alpha'-W_0)^{-1/4}\exp[i\int^x(\alpha'-W_0)^{1/2}dx']$ where α' is the initial prediction for α as determined by $\int_0^{\pi}(\alpha'-W_0)^{1/2}dx=\nu\pi$) renders the excellent value of 0.0895063.

III. FRÖMAN AND FRÖMAN'S EXPANSION

As a comparison, let us examine a different expansion for higher order terms for the phase integral derived by Fröman and Fröman.[4] For Fröman and Fröman's expansion of order $2M+1$, the quantization for the lattice potential appearing in Mathieu's equation is

$$\int_0^{\pi}\sum_{n=0}^{M}Y_{2n}\,Q(x)\,dx=\nu\pi,\quad|\nu|\neq 1,2,3,\cdots,$$

where $Q(x)=(\alpha-2\gamma\cos 2x)^{1/2}$ and the Y_{2n}'s are the expansion terms. For the particular case of the lattice potential appearing in Mathieu's equation $Y_0=1$,

$$Y_2=\frac{\gamma}{Q^4}\left(-\cos 2x+\frac{\gamma}{Q^2}\frac{5}{2}\sin^2 2x\right.,$$

$$Y_4=\frac{\gamma}{Q^6}\left\{-\cos 2x+\frac{\gamma}{Q^2}\left[14\sin^2 2x-9.5\cos^2 2x\right.\right.$$

TABLE II. Calculated eigenvalues, α's, of Mathieu's equation, $\psi''+(\alpha-2\gamma\cos 2x)\psi=0$ for selected γ and selected values of the characteristic exponent ν and various truncations of order $2M+1$ for Fröman and Fröman's expansion of phase integral.

Characteristic exponent, ν		0.3	3.5	4.5	5.5
γ		0.03	1.0	1.0	1.0
α	Rounded-off exact	0.0895	12.294632	20.27600336	30.26710156
α	$M=0$ [a]	0.0952	12.290901	20.27471022	30.26653458
α	$M=1$	0.1272	12.294291	20.27593723	30.26708253
α	$M=2$	*	12.294591	20.27599963	30.26710089

* Outside domain of validity of algorithm.

[a] For $M=0$, the expansion truncates to the WKB approximation.

$$+\frac{\gamma}{Q^2}\,(110.5\sin^2 2x\cos 2x+\frac{\gamma}{Q^2}\,138.125\sin^4 2x\Big]\Big\},$$

. . . .

Table II exhibits the computed energy levels (i.e., eigenvalues) for various orders $2M+1$ of Fröman and Fröman's expansion for the same parametric pairs (γ, ν) as in Table I. In the case of long wavelengths (e.g., $\nu=0.3$), Fröman and Fröman's expansion is divergent as the Y_{2n}'s form series of inverse higher-order Q terms. In fact, the algorithm for computing α is outside its domain of validity at $\nu=0.3$ for $M=2$. Furthermore for $M=0$, Fröman and Fröman's method has the same restriction to short wavelengths as the WKB method. In contrast, Table I shows good convergence for the modified potential expansion in the long wavelength case since the singular points of the modified potential expansion are the centers of the various band gaps.

For moderately short wavelength cases represented by $\nu=3.5$, 4.5, 5.5 with $\gamma=1$ of Tables I and II, the action-variable computations for α with the two expansions exhibit accuracy of comparable order. Nevertheless, for $|\gamma| \ll 1$ and for short wavelengths, the modified potential expansion has the advantage with respect to the expansion of Fröman and Fröman since in the latter expansion $Y_{2n}=O(\gamma)$ for $n \geq 1$ while in the former expansion $W_n=O(\gamma^{n+1})$. Thus, in the limit that $\gamma \to 0$, the modified potential expansion has better convergence. As the representations for an effective action variable that are formed by the two different expansions appear to be the analytic continuation of each other by correlating coefficients of γ^n between the two truncated series, different domains of convergence for the two expansions are expected.

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[2]E.R. Floyd, J. Acoust. Soc. Am. **60**, 801—09 (1976).
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On nonlinear transformations for time-dependent polynomial Hamiltonians

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A formal method is demonstrated for the transformation of polynomial Hamiltonians with time-dependent coefficients to time-independent polynomial Hamiltonians. The transformation functions are themselves polynomials in the canonical variables with time-dependent coefficients. These coefficients are determined by sets of first order linear differential equations. The results apply equally well to multidimensional problems. The work is a generalization of the author's earlier work on time-dependent linear transformations for quadratic Hamiltonians.

1. INTRODUCTION

In recent years there has been considerable interest in time-dependent oscillator systems with Hamiltonians of the type

$$H(q,p,t)=\sum_{j=0}^{2} A_j(t)q^j p^{2-j}. \tag{1.1}$$

The basic interest has been in finding an invariant for the motion described by H (1.1). In essence there have been two approaches. The first, based on the work of Kruskal,[1] was followed by Lewis,[2] Symon,[3] and Sarlet.[4] The second, more recent approach, uses time-dependent linear canonical transformations. The work of Günther and Leach[5] and Leach[6-9] on this subject has given a reasonable physical basis to the problem of finding an invariant. It ought to be noted that the results apply equally well to the general $2n$-dimensional quadratic Hamiltonian.

Hamiltonians of the type (1.1) have been of practical interest mainly in the discussion of a particle moving in an electromagnetic field, for examle in the work of Courant[10] and Seymour.[11] As a quadratic Hamiltonian usually arises as a first approximation to a more complex system, it is not surprising that there is now an interest in the time-dependent anharmonic oscillator. Without specifying the nature of the anharmonicity, the problem becomes the study of a time-dependent polynomial Hamiltonian.

The study of polynomial Hamiltonians has long been of interest in the field of celestial mechanics, as witness the work of Cherry.[12] There the problem is usually referred to as the motion of a particle about a singular or equilibrium point. The method of attack has been to transform the Hamiltonian to a normal form for which integrals are obvious. The canonical transformations are of polynomial form and problems of convergence arise. It is usual to discuss the problem in a formal way to demonstrate the possibility, if not the actuality, of a solution. Gustavson[13] has found that a truncated transformation gives useful results in computer applications.

The problem which we study in this paper is thus both old and new, depending upon the area of application. We shall demonstrate that a time-dependent polynomial Hamiltonian may be transformed formally to any other polynomial Hamiltonian (which may be time-dependent). The idea of the equivalence of any two Hamiltonians of the same number of degrees of freedom is not new (cf. Kohler[14]), but there does not appear to have been an explicit treatment of the actual transformations involved.

For the time-dependent problem, the usual approach has been to use a time-independent generating function. We shall show that a time-dependent generating function may be constructed for the time-dependent problem. In fact a time-dependent generating function may be used for both classes of problem, but is of particular relevance to time-dependent problems. The generating function method has the drawback of not providing explicit formulas for the new coordinates in terms of the old or vice versa. We shall show that it is possible to approach the problem in such a way that explicit formulas are available. We believe that this represents a considerable improvement. As the algebra is tedious, most of our discussion will deal with the Hamiltonian of a one-dimensional system. There will be an extension of the discussion to multidimensional systems sufficient to indicate the generality of our results.

2. ONE-DIMENSIONAL PROBLEM: TRANSFORMATION OF THE QUADRATIC TERMS

The general polynomial Hamiltonian describing the motion of a one-dimensional system about a singular point is

$$H(q,p,t)=\sum_{r=2}^{\infty}\sum_{j=0}^{r} A_j^r(t)q^j p^{r-j}, \tag{2.1}$$

where (q,p) are the canonically conjugate coordinates and the coefficients $A_j^r(t)$ are real continuous functions of time. The possible existence of a coordinate-free term in (2.1) has no bearing on the motion and is ignored. We assume that $H(q,p,t)$ is finite for all t and finite (q,p).

We separate out the quadratic terms in (2.1) by writing

$$H(q,p,t)=\sum_{j=0}^{2} A_j^2 q^j p^{2-j}+\sum_{r=3}^{\infty}\sum_{j=0}^{r} A_j^r q^j p^{r-j}. \tag{2.2}$$

The quadratic part may be written in matrix form as

$$H^{(2)}(q,p,t)=\tfrac{1}{2}[q,p]M\begin{bmatrix} q \\ p \end{bmatrix}, \tag{2.3}$$

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where the 2×2 matrix M is given by

$$M=\begin{bmatrix}2A_2^2, & A_1^2\\ A_1^2, & 2A_0^2\end{bmatrix} \tag{2.4}$$

The quadratic part $H^{(2)}(q,p,t)$ may be transformed to (cf. Leach[7])

$$\bar{H}^{(2)}(Q,P,t)=\tfrac{1}{2}[Q,P]\bar{M}\begin{bmatrix}Q\\P\end{bmatrix} \tag{2.5}$$

by means of the linear transformation

$$\begin{bmatrix}Q\\P\end{bmatrix}=S\begin{bmatrix}q\\p\end{bmatrix}. \tag{2.6}$$

The transformation matrix S satisfies the first-order differential equation.

$$\dot{S}=J\bar{M}S-SJM \tag{2.7}$$

where J is the 2×2 sympletic matrix. The transformation is canonical provided

$$SJS^T=J. \tag{2.8}$$

(For a proof that this is always possible, see Leach.[7] The discussion in Sec. 7 is a generalization of the result.)

The equation (2.7) has a solution provided the elements $\bar{M}$ and M are continuous functions of time (cf. Ince,[15] pp. 71,72). In particular we may choose $\bar{M}$ to be a matrix with constant elements. The generating function of the transformation is quadratic and so does not affect the higher terms in $H(q,p,t)$. Thus, after the transformation (2.6), we have

$$\bar{H}(Q,P,t)=\bar{H}^{(2)}(Q,P)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)\times(S_4Q-S_2P)^j(-S_3Q+S_1P)^{r-j}, \tag{2.9}$$

where $H^{(2)}(Q,P)$ has constant coefficients and

$$S=\begin{bmatrix}S_1 & S_2\\ S_3 & S_4\end{bmatrix}. \tag{2.10}$$

As the summed part of (2.9) is of minimum degree three, the transformation of $H(q,p,t)$ (2.1) may be discussed in terms of the transformation of

$$H(q,p,t)=H^{(2)}(q,p)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)q^jp^{r-j}. \tag{2.11}$$

We have emphasized this point because of the advantage it gives us in later work. The systems of differential equations which arise from (2.11) are linear, whereas those which would have been obtained had we used (2.1) are nonlinear. The reason for this is that, in the case of (2.11), it is suitable to choose $\bar{H}$ such that $\bar{H}^{(2)}(Q,P)$ has the same functional form as $H^{(2)}(q,p)$ and so the first term of the transformation is simply the identity. As is explained in Sec. 4, by starting with the identity, the nonlinear terms in any system of differential equations belong to lower order coefficients than those which the system is determining.

3. TRANSFORMABILITY OF HIGHER ORDER TERMS INDUCTIVE PROOF

We assume now that the coefficients of all terms up to order n ($\geqslant2$) have been rendered constant by a series of suitable transformations. We write

$$H(q,p,t)=H^{(n)}(q,p)+\sum_{j=0}^{n+1}A_j^{n+1}(t)\times q^jp^{n+1-j}+R(q,p,t), \tag{3.1}$$

where $H^{(n)}(q,p)$ has constant coefficients and contains all terms of order $\leqslant n$ while $R(q,p,t)$ contains all terms of order $>(n+1)$. For the purposes of this discussion we use the type two generating function $F_2(q,P,t)$ so that

$$p=\frac{\partial F_2(q,P,t)}{\partial q},\qquad Q=\frac{\partial F_2(q,P,t)}{\partial P}. \tag{3.2}$$

Writing

$$F_2(q,P,t)=qP+\sum_{k=0}^{n+1}B_k(t)q^kP^{n+1-k}, \tag{3.3}$$

$$\bar{H}(q,P,t)=H^{(n)}\left(q,\frac{\partial F_2}{\partial q}\right)+\sum_{j=0}^{n+1}A_j^{n+1}(t)q^j\times\left(P+\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}\right)^{n+1-j}+R\left(q,\frac{\partial F_2}{\partial q}\right)+\sum_{k=0}^{n+1}\dot{B}_k(t)q^kP^{n+1-k}. \tag{3.4}$$

Consider any term in $H^{(n)}(q,p)$, say $C_l^rq^lp^{r-l}$ where $0\leqslant l\leqslant r$, $2\leqslant r\leqslant n$. Since

$$p=P+\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}, \tag{3.5}$$

$$Q=q+\sum_{k=0}^{n+1}(n+1-k)B_k(t)q^kP^{n-k},$$

$$C_l^rq^lp^{r-l}=C_l^r\left[Q-\sum_{k=0}^{n+1}(n+1-k)B_k(t)q^kP^{n-k}\right]^l\times\left[P+\sum_{m=0}^{n+1}mB_m(t)q^{m-1}P^{n+1-m}\right]^{r-l}$$

$$=C_l^rQ^lp^{r-l}+\text{other terms}. \tag{3.6}$$

Ignoring coefficients and considering only the powers of Q,

P, and q, a typical example of the other terms will be

$$Q^{l-i}\,[q^k P^{n-k}]^i P^{r-l-j}\,[q^{m-1}P^{n+1-m}]^j, \tag{3.7}$$

where $0\leqslant i\leqslant l$, $0\leqslant j\leqslant r-l$, and $i+j\geqslant 1$ [since $i+j=0$ is covered by the first term of (3.6)]. Again making use of (3.5), the leading term in (Q,P) is of degree

$$l-i+i(k+n-k)+r-l-j+j(m-1+n+1-m)$$
$$\Longleftrightarrow (i+1)(n-1)+r\geqslant n-1+2=n+1$$

since $r\geqslant 2$ and $i+j\geqslant 1$. Hence $H^{(n)}(q,p)$ is transformed to $H^{(n)}(Q,P)$ plus possible terms of degree $\geqslant(n+1)$, where $H^{(n)}(Q,P)$ has the same functional form as $H^{(n)}(q,p)$.

We may write (3.4) as

$$\begin{aligned}\bar H(q,P,t)=&\sum_{r=2}^{n}\sum_{j=0}^{n}C_j^r q^j\\ &\times\Big[P+\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}\Big]^{r-j}\\ &+\sum_{j=0}^{n+1}A_j^{n+1}(t)q^j\\ &\times\Big[P+\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}\Big]^{n+1-j}\\ &+R(q,P,t)+\sum_{k=0}^{n+1}\dot B_k(t)q^kP^{n+1-k}.\end{aligned}\tag{3.8}$$

As we are seeking an $\bar H$ of the form

$$\bar H(Q,P,t)=\sum_{r=2}^{n+1}\sum_{j=0}^{r}C_j^rQ^jP^{r-1}+\bar R(Q,P,t),\tag{3.9}$$

where $\bar R$ contains the terms of degree $>(n+1)$, we have in terms of q,P,t,

$$\begin{aligned}&\bar H(q,P,t)\\ &=\sum_{r=2}^{n+1}\sum_{j=0}^{r}C_j^r\Big[q+\sum_{k=0}^{n+1}(n+1-k)B_k(t)q^kP^{r-k}\Big]^jP^{r-j}\\ &\quad+\bar R(q,P,t).\end{aligned}\tag{3.10}$$

Extracting the terms of degree $(n+1)$ from (3.8) and (3.10), the desired result is achieved provided

$$\begin{aligned}&C_1^2q\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}+2C_0^2\\ &\times P\sum_{k=0}^{n+1}kB_k(t)q^{k-1}P^{n+1-k}\\ &+\sum_{j=0}^{n+1}A_j^{n+1}(t)q^jP^{n+1-j}+\sum_{k=0}^{n+1}\dot B_k(t)q^kP^{n+1-k}\\ &=\sum_{k=0}^{n+1}C_k^{n+1}q^kP^{n+1-k}+C_1^2\\ &\times P\sum_{k=0}^{n+1}(n+1-k)B_k(t)q^kP^{n-k}\\ &+2C_2^2q\sum_{k=0}^{n+1}(n+1-k)B_k(t)q^kP^{n-k}.\end{aligned}\tag{3.11}$$

On equating coefficients, we obtain the system of linear first-order differential equations

$$\begin{aligned}&\dot B_k(t)+C_1^2kB_k(t)+2C_0^2(k+1)B_{k+1}(t)\\ &\quad-C_1^2(n+1-k)B_k(t)-2C_2^2(n+2-k)B_{k-1}(t)\\ &\quad=C_k^{n+1}-A_k^{n+1}(t),\quad 1\leqslant k\leqslant n,\\ &\dot B_0(t)+2C_0^2B_1(t)-(n+1)C_1^2B_0(t)=C_0^{n+1}-A_0^{n+1}(t),\\ &\dot B_{n+1}(t)+(n+1)C_0^2B_{n+1}(t)-2C_2^2B_n(t)\\ &\quad=C_{n+1}^{n+1}-A_{n+1}^{n+1}(t).\end{aligned}\tag{3.12}$$

This system has a solution since the A's were specified as continuous. Clearly the choice of the C's is arbitrary.

Thus we have the formal result that, by a process of successive canonical transformations, $H(q,p,t)$ may be transformed to $\bar H(Q,P)$.

4. SINGLE GENERATING FUNCTION METHOD

From the foregoing it is evident that the formal transformation from $H(q,p,t)$ to an arbitrary $\bar H(Q,P)$ can be accomplished by a means of succession of polynomial generating functions. The process may be achieved in one step by a single suitable generating function. The coefficients of the polynomial generating function are obtained in the following manner.

We saw in Sec. 2 that the original Hamiltonian may be written, without loss of generality, as

$$H(q,p,t)=H^{(2)}(q,p)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)q^{r-j}p^j.\tag{4.1}$$

The transformed Hamiltonian is

$$\bar H(Q,P)=H^{(2)}(Q,P)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}C_j^rQ^jP^{r-j}.\tag{4.2}$$

It is convenient to write

$$\begin{aligned}H^{(2)}(q,p)&=\sum_{j=0}^{2}A_j^2q^{2-j}p^j,\\ H^{(2)}(Q,P)&=\sum_{j=0}^{2}C_j^2Q^jP^{2-j}.\end{aligned}\tag{4.3}$$

Since the functional forms of $H^{(2)}(q,p)$ and $H^{(2)}(Q,P)$ are identical, the coefficients are related by

$$A_0^2=C_2^2,\quad A_1^2=C_1^2,\quad A_2^2=C_0^2.\tag{4.4}$$

We propose the type two generating function

$$F_2(q,P,t)=qP+\sum_{r=3}^{\infty}\sum_{j=0}^{r}B_j^r(t)q^jP^{r-j}\tag{4.5}$$

$$Q=q+\sum_{r=3}^{\infty}\sum_{j=0}^{r}(r-j)B_j^r(t)q^jP^{r-1-j},$$

$$\Leftrightarrow \tag{4.6}$$

$$p=P+\sum_{r=3}^{\infty}\sum_{j=0}^{r}jB_j^r(t)q^{j-1}P^{r-j}$$

The standard transformation equation

$$\bar{H}(q,P,t)=H(q,P,t)+\frac{\partial F_2(q,P,t)}{\partial t} \tag{4.7}$$

becomes

$$\sum_{r=3}^{\infty}\sum_{j=0}^{r}\dot{B}_j^r(t)q^jP^{r-j}+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)q^{r-j}\times\left[P+\sum_{s=3}^{\infty}\sum_{i=0}^{s}iB_i^s(t)q^{i-1}p^{s-i}\right]^j$$

$$+\sum_{j=0}^{2}A_j^2q^{2-j}\left[P+\sum_{s=3}^{\infty}\sum_{i=0}^{s}iB_i^s(t)q^{i-1}P^{s-i}\right]^j$$

$$=\sum_{r=3}^{\infty}\sum_{j=0}^{r}C_j^r$$

$$\times\left[q+\sum_{s=3}^{\infty}\sum_{i=0}^{s}(s-i)B_i^s(t)q^iP^{s-1-i}\right]^jP^{r-j}$$

$$+\sum_{j=0}^{2}C_j^2$$

$$\times\left[q+\sum_{s=3}^{\infty}\sum_{i=0}^{s}(s-i)B_i^s(t)q^iP^{s-1-i}\right]^jP^{2-j}. \tag{4.8}$$

The quadratic terms cancel. Collecting the cubic terms, we have

$$\sum_{j=0}^{3}\dot{B}_j^3(t)q^jP^{3-j}+\sum_{j=0}^{3}A_j^3(t)q^{3-j}P^j$$

$$+A_1^2q\sum_{j=0}^{3}jB_j^3(t)q^{j-1}P^{3-j}$$

$$+2A_2^2P\sum_{j=0}^{3}jB_j^3(t)q^{j-1}P^{3-j}$$

$$=\sum_{j=0}^{3}C_j^3q^jP^{3-j}+C_1^2P$$

$$\times\sum_{j=0}^{3}(3-j)B_j^3(t)q^jP^{2-j}$$

$$+2C_2^2q\sum_{j=0}^{3}(3-j)B_j^3(t)q^jP^{2-j}. \tag{4.9}$$

Equating coefficients of like powers to zero, we obtain

$$\begin{bmatrix} D-3C_1^2, & 2A_2^2, & 0, & 0 \\ -6C_2^2, & D+A_1^2-2C_1^2, & 4A_2^2, & 0 \\ 0, & -4C_2^2, & D+2A_1^2-C_1^2, & 6A_2^2 \\ 0, & 0, & -2C_2^2, & D+3A_1^2 \end{bmatrix}\begin{bmatrix} B_0^3 \\ B_1^3 \\ B_2^3 \\ B_3^3 \end{bmatrix}=\begin{bmatrix} C_0^3-A_3^3 \\ C_1^3-A_2^3 \\ C_2^3-A_1^3 \\ C_3^3-A_0^3 \end{bmatrix}, \tag{4.10}$$

where $D=d/dt$. This is linear in the B's and, given the continuity of the A's, the system has a unique solution set.

The process of finding the B's will always involve the solution of an equation linear in the unknown B's. From (4.8) we see that there are terms which are nonlinear in the B's. However, when such a nonlinear term appears in a differential equation, it will be as a known function. For example, we look at the degree of the term with coefficient $(B_j^3)^2$ in the second term of (4.8). It is $r+2\geqslant 5$. The first set of equations containing such a term would be that which determines B_j^5.

5. DIRECT TRANSFORMATION APPROACH: FORWARD METHOD

Although the generating function approach is of theoretical value in approaching the problem, there remains the difficulty of inverting the function to obtain q and p in terms of Q and P. The presence of explicit time dependence in the generating function makes the use of computer inversion prohibitive. An alternative approach is to define q and p as explicit polynomials in Q and P with time-dependent coefficients.

The Hamiltonians $H(q,p,t)$ and $\bar{H}(Q,P)$ may of course be arbitrary polynomials of degree greater than or equal to two. To illustrate the method, we take

$$H(q,p,t)=\tfrac{1}{2}(q^2+p^2)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)q^{r-j}p^j, \tag{5.1}$$

$$\bar{H}(Q,P)=\tfrac{1}{2}(Q^2+P^2). \tag{5.2}$$

In view of our earlier work there is no real loss of generality. The canonical variables q and p are given formally by

$$q=Q+\sum_{r=2}^{\infty}\sum_{j=0}^{r}B_j^r(t)Q^jP^{r-j}, \tag{5.3}$$

$$p=P+\sum_{r=2}^{\infty}\sum_{j=0}^{r}C_j^r(t)Q^jP^{r-j}. \tag{5.4}$$

We require the description of the motion by H and $\bar{H}$ to be equivalent. Differentiation (5.3) and (5.4) with respect to

time and substituting for $\dot{q}, \dot{p}, \dot{Q}$, and $\dot{P}$ from Hamilton's equations for H and $\bar{H}$, we have

$$p+\sum_{r=3}^{\infty}\sum_{j=0}^{r} jA_j^r q^{r-j}p^{j-1} = P+\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{\dot{B}_j^r Q^j P^{r-j}+jB_j^r Q^{j-1}P^{r+1-j} -(r-j)B_j^r Q^{j+1}P^{r-1-j}\}, \tag{5.5}$$

$$q+\sum_{r=3}^{\infty}\sum_{j=0}^{r}(r-j)A_j^r q^{r-1-j}p^j = Q+\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{-\dot{C}_j^r Q^j P^{r-j}-jC_j^r Q^{j-1}P^{r+1-j} +(r-j)C_j^r Q^{j+1}P^{r-1-j}\}. \tag{5.6}$$

Making use of (5.3) and (5.4) in the left sides of (5.5) and (5.6) we have the equations in terms of Q and P

$$\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{\dot{B}_j^r Q^j P^{r-j}+jB_j^r Q^{j-1}P^{r+1-j} -(r-j)B_j^r Q^{j+1}P^{r-1-j}-C_j^r Q^j P^{r-j}\} = \sum_{r=3}^{\infty}\sum_{j=0}^{r} jA_j^r\left\{Q+\sum_{s=0}^{\infty}\sum_{i=0}^{s}B_i^s Q^i P^{s-i}\right\}^{r-j} \times\left\{P+\sum_{u=2}^{\infty}\sum_{l=0}^{u}C_l^u Q^l P^{u-l}\right\}^{j-1}, \tag{5.7}$$

$$\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{\dot{C}_j^r Q^j P^{r-j}+jC_j^r Q^{j-1}P^{r+1-j} -(r-j)C_j^r Q^{j+1}P^{r-1-j}+B_j^r Q^j P^{r-j}\} = -\sum_{r=3}^{\infty}\sum_{j=0}^{r}(r-j)A_j^r\left\{Q+\sum_{s=2}^{\infty}\sum_{i=0}^{s}B_i^s Q^i P^{s-i}\right\}^{r-1-j} \times\left\{P+\sum_{u=2}^{\infty}\sum_{l=0}^{u}C_l^u Q^l P^{u-l}\right\}^{j}. \tag{5.8}$$

Separation of the coefficients of like terms in Q and P from (5.7) and (5.8) will yield systems of linear differential equations for the coefficients $B_j^r(t)$ and $C_j^r(t)$. The form of these equations is

$$M_n\mathbf{x}^n=\mathbf{f}(A_j^r,B_i^s,C_l^u), \tag{5.9}$$

where

$$\mathbf{x}^n=\begin{bmatrix}\mathbf{B}^n\\ \mathbf{C}^n\end{bmatrix}, \quad M_n=\begin{bmatrix}K_n & -I\\ I & K_n\end{bmatrix}$$

$$K_n=\begin{bmatrix} D & 1 & 0 & \cdots & & & \\ -n & D & 2 & \cdots & & & \\ 0 & -(n-1) & D & \cdots & & & \\ \cdot & \cdot & \cdot & \cdots & D & n-1 & 0\\ \cdot & \cdot & \cdot & \cdots & -2 & D & n\\ & & & & 0 & -1 & D\end{bmatrix}$$

and $D=d/dt$. The nonhomogeneous term denoted by $\mathbf{f}(A_j^r,B_i^r,C_l^u)$ is not necessarily linear in the B's and C's. As $r\leqslant n$, $s<n$, and $u<n$, this does not affect the linearity of the differential equation.

The requirement that the transformation be canonical imposes a set of constraints on the B's and C's. A full discussion of these constraints will be given in Sec. 7. At the moment it is sufficient to note that the constraints cause no difficulty.

6. DIRECT TRANSFORMATION APPROACH: BACKWARDS METHOD

If, instead of writing

$$q=q(Q,P,t), \quad p=p(Q,P,t) \tag{6.1}$$

as in Sec. 5, we write

$$Q=Q(q,p,t), \quad P=P(q,p,t), \tag{6.2}$$

it will be possible to express $\bar{H}$ in terms of q, p, and t. Since we choose $\bar{H}$ to be constant, $\bar{H}(q,p,t)$ will be an invariant of the motion described by H (cf. Leach[9] for the linear transformation case).

For the purposes of our discussion we shall use the Hamiltonians

$$H=\tfrac{1}{2}(q^2+p^2)+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)q^j p^{r-j}, \tag{6.3}$$

$$\bar{H}=\tfrac{1}{2}(Q^2+P^2). \tag{6.4}$$

We express the transformation as

$$Q=q+\sum_{r=2}^{\infty}\sum_{j=0}^{r}B_j^r(t)q^j p^{r-j}, \tag{6.5}$$

$$P=p+\sum_{r=2}^{\infty}\sum_{j=0}^{r}C_j^r(t)q^j p^{r-j}. \tag{6.6}$$

Following the same lne of argument as in Sec. 5, we obtain the following equations in q and p.

$$\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{\dot{B}_j^r q^j p^{r-j}+jB_j^r q^{j-1}p^{r+1-j} -(r-j)B_j^r q^{j+1}p^{r-1-j}-C_j^r q^j p^{r-j}\} = -\sum_{r=3}^{\infty}\sum_{j=0}^{r}(r-j)A_j^r q^j p^{r-1-j} +\sum_{r=2}^{\infty}\sum_{j=0}^{r}B_j^r\sum_{s=3}^{\infty}\sum_{i=0}^{s}A_i^s(js-ir) \times q^{i+j-1}p^{r+s-i-j-1}, \tag{6.7}$$

$$\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{\dot{C}_j^r q^j p^{r-j}+jC_j^r q^{j-1}p^{r+1-j} -(r-j)C_j^r q^{j+1}p^{r-1-j}+B_j^r q^j p^{r-j}\} = \sum_{r=3}^{\infty}\sum_{j=0}^{r}jA_j^r q^{j-1}p^{r-j}$$

$$+\sum_{r=2}^{\infty}\sum_{j=0}^{r} C_j^r \sum_{s=3i=0}^{\infty}\sum_{i=0}^{s} A_i^s(js-ir)$$

$$\times q^{i+j-1}p^{r+s-i-j-1}. \tag{6.8}$$

These equations are similar to those of (5.7) and (5.8). The structure is simpler because the ultimate terms in each are not as complex as before. Separation of the coefficients of like terms in q and p from (6.7) and (6.8) will led to systems of linear differential equations for the coefficients $B_j^r(t)$ and $C_j^r(t)$. The form of these equations is the same as (5.9), the equations being

$$\dot{B}_k^m = -(k+1)\,B_{k+1}^m + (m+1-k)B_{k-1}^m + C_k^m$$

$$-(m+1-k)A_k^{m+1} - \sum_{\Gamma}(lu-pv)\,B_l^v A_p^u, \tag{6.9}$$

$$\dot{C}_k^m = -(k+1)\,C_{k+1}^m + (m+1-k)C_{k-1}^m - B_k^m$$

$$+(k+1)\,A_{k+1}^{m+1} - \sum_{\Gamma}(lu-pv)\,C_l^v A_p^u. \tag{6.10}$$

The summation denoted by Σ_Γ is over those terms for which

$$l+p=k+1, \quad u+v=m+2. \tag{6.11}$$

7. THE REQUIREMENT OF CANONICITY

When the generating function approach is used, the transformation is automatically canonical. This is not the case with the direct transformation approaches. We must impose the condition that the Poisson Bracket of the transformation be unity. In this section we establish the constraints on the B's and C's for the transformation to be canonical and prove that these constraints hold for all time. Before proceeding to a general proof, we look at two simple examples to illustrate the principle of the proof. For the purposes of the discussion, we use the transformations of Sec. 6.

Taking the Poisson Bracket of Q and P with respect to q and p, the transformation defined by (6.5) and (6.6) is canonical provided

$$\sum_{r=2}^{\infty}\sum_{j=0}^{r}\{jB_j^r q^{j-1}p^{r-j} + (r-j)C_j^r q^j p^{r-1-j}\}$$

$$+\sum_{r=2}^{\infty}\sum_{s=2}^{\infty}\sum_{j=0}^{r}\sum_{i=0}^{s}(js-ir)$$

$$\times B_j^r C_i^s q^{i+j-1}p^{r+s-i-j-1} = 0. \tag{7.1}$$

For example, a comparison of the linear and quadratic terms imposes the requirements that

$$B_1^2 + 2C_0^2 = 0,$$

$$2B_2^2 + C_1^2 = 0, \tag{7.2}$$

$$B_1^3 + 3C_0^3 + 2\{B_1^2 C_0^2 - B_0^2 C_1^2\} = 0,$$

$$2B_2^3 + 2C_1^3 + 4\{B_2^2 C_0^2 - B_0^2 C_2^2\} = 0, \tag{7.3}$$

$$3B_3^3 + C_0^3 + 2\{B_2^2 C_1^2 - B_1^2 C_2^2\} = 0.$$

The sets of equations satisfied by the B^2's, C^2's, B^3's and C^3's are, respectively,

$$\left[\begin{array}{ccc|ccc} D & 1 & 0 & -1 & 0 & 0 \\ -2 & D & 2 & 0 & -1 & 0 \\ 0 & -1 & D & 0 & 0 & -1 \\ \hline 1 & 0 & 0 & D & 1 & 0 \\ 0 & 1 & 0 & -2 & D & 2 \\ 0 & 0 & 1 & 0 & -1 & D \end{array}\right]\left[\begin{array}{c} B_0^2 \\ B_1^2 \\ B_2^2 \\ \hline C_0^2 \\ C_1^2 \\ C_2^2 \end{array}\right] = \left[\begin{array}{c} -3A_0^3 \\ -2A_1^3 \\ -A_2^3 \\ \hline A_1^3 \\ 2A_2^3 \\ 3A_3^3 \end{array}\right], \tag{7.4}$$

$$\left[\begin{array}{cccc|cccc} D & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ -3 & D & 2 & 0 & 0 & -1 & 0 & 0 \\ 0 & -2 & D & 3 & 0 & 0 & -1 & 0 \\ 0 & 0 & -1 & D & 0 & 0 & 0 & -1 \\ \hline 1 & 0 & 0 & 0 & D & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -3 & D & 2 & 0 \\ 0 & 0 & 1 & 0 & 0 & -2 & D & 3 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & D \end{array}\right]\left[\begin{array}{c} B_0^3 \\ B_1^3 \\ B_2^3 \\ B_3^3 \\ \hline C_0^3 \\ C_1^3 \\ C_2^3 \\ C_3^3 \end{array}\right]$$

$$= \left[\begin{array}{c} -4A_0^4 \\ -3A_1^4 \\ -2A_2^4 \\ -A_3^4 \\ \hline A_1^4 \\ 2A_2^4 \\ 3A_3^4 \\ 4A_4^4 \end{array}\right] + \left[\begin{array}{c} 2B_0^2A_1^3 - 3B_1^2A_0^3 \\ 4B_0^2A_2^3 - B_1^2A_1^3 - 6B_2^2A_0^3 \\ 6B_0^2A_3^3 + B_1^2A_2^3 - 4B_2^2A_1^3 \\ 3B_1^2A_3^3 - 2B_2^2A_2^3 \\ \hline 2C_0^2A_1^3 - 3C_1^2A_0^3 \\ 4C_0^2A_2^3 - C_1^2A_1^3 - 6C_2^2A_0^3 \\ 6C_0^2A_3^3 + C_1^2A_2^3 - 4C_2^2A_1^3 \\ 3C_1^2A_3^3 - 2C_2^2A_2^3 \end{array}\right]. \tag{7.5}$$

For the transformation to be canonical, the constraints (7.2) and (7.3) must be consistent with the solutions of (7.4) and (7.5). The general solution set of (7.4) depends upon six arbitrary constants and it is possible to select them such that, at some time t_0, the two constraints (7.2) are satisfied. Let

$$x_1=B_1^2+2C_0^2, \quad x_2=2B_2^2+C_1^2. \tag{7.6}$$

From (7.4) we see that

$$\dot{x}_1=-x_2, \quad \dot{x}_2=x_1. \tag{7.7}$$

Considered as a system of equations, (7.7) has a singular point at (0,0). Thus, if the constraints are satisfied at $t=t_0$, they are satisfied for all t. Similarly, writing x_1, x_2, and x_3 for the left-hand terms in (7.3) and using (7.5), we have

$$\dot{x}_1=-x_2, \quad \dot{x}_2=2x_1-2x_3, \quad \dot{x}_3=x_2. \tag{7.8}$$

The point (0,0,0) is a singular point and, if the constraints (7.3) are satisfied at $t=t_0$, they are satisfied for all time.

The purpose of the two examples given above was to illustrate the principle of the proof of the general result. From (7.1) the coefficient of $q^{k-1}p^{m-k}$ is extracted and we write

$$x_k^m+kB_k^m+(m+1-k)C_{k-1}^m+\sum_2(lu-pv)B_l^vC_p^u. \tag{7.9}$$

The summation denoted by Σ_2 is over those terms for which

$$l+p=k, \quad u+v=m+1. \tag{7.10}$$

Using the differential equations (6.9) and (6.10) we find, after some algebra and careful attention to the summation limits, that

$$\dot{x}_k^m=-kx_{k+1}^m+(m+1-k)x_{k-1}^m$$

$$-\sum_2(js-ir)x_{j+1}^{r+1}A_i^s, \tag{7.11}$$

where we have adopted the convention that $x_k^m\equiv 0$ for $k<0$ and $k>m$. The x's in the summation are of lower order than x^m since $s\geqslant 3$. The system of equations represented by (7.11) has a singular point at $t=t_0$ if the constraints $x_k^m(t_0)=0$ are applied. Thus the constraints hold for all time.

We see that that the transformation defined by Eqs. (6.5) and (6.6) is canonical under the constraints given above. The transformation defined by Eqs. (5.3) and (5.4) may be treated similarly.

8. MULTIDIMENSIONAL PROBLEM

It has long been held that commensurability between the coefficients of the quadratic parts of the Hamiltonian describing a higher dimensional problem prevents the transformation of a polynomial Hamiltonian to one of normal form. We propose that this is not the case since the Hamiltonians

$$H^{(2)}(q,p)=\tfrac{1}{2}\sum_i(q_i^2+p_i^2) \quad \left(\text{or } \sum_i q_ip_i\right), \tag{8.1}$$

$$H^{(2)}(Q,P)=\tfrac{1}{2}\sum_i C^i(Q_i^2+P_i^2) \quad \left(\text{or } \sum_i C^iQ_iP_i\right), \tag{8.2}$$

where the C's are incomensurable, are equivalent under a time-dependent linear transformation.

The generalization of the work on the one-dimensional problem to many dimensions is mainly a matter of coping with increasingly complex algebra except for one feature. The problem of commensurability has in the past lead to the vanishing of coefficients of some of the terms in the transformation so that they could not be determined. We shall show that every such coefficient occurs as its derivative with nonvanishing coefficient. That this will be the case for each of the three approaches used in the one-dimensional problem is not surprising.

We do not intend to labor the point with algebra of meaningless and repetitive complexity. Consequently, we indicate the approaches for the case of the Hamiltonian of a two-dimensional motion.

9. COEFFICIENTS OF THE GENERATING FUNCTION

As a linear transformation may be used to convert the coefficients of the quadratic terms to constants, we assume them constant and of the desired form. The Hamiltonian is taken to be

$$H(q_1,q_2,p_1,p_2,t)$$

$$=\sum_{j=0}^{2}A_j^{2,0}q_1^{2-j}p_1^j+\sum_{j=0}^{2}A_j^{0,2}q_2^{2-j}p_2^j$$

$$+\sum_{r_1+r_2=3}^{\infty}\sum_{j_1=0}^{r_1}\sum_{j_2=0}^{r_2}A_{j_1j_2}^{r_1r_2}(t)q_1^{r_1-j_1}q_2^{r_2-j_2}p_1^{j_1}p_2^{j_2}. \tag{9.1}$$

The transformed Hamiltonian is

$$\bar{H}(Q_1,Q_2,P_1,P_2,t)$$

$$=\sum_{j=0}^{2}C_j^{2,0}Q_1^jP_1^{2-j}+\sum_{j=0}^{2}C_j^{0,2}Q_2^jP_2^{2-j}$$

$$+\sum_{r_1+r_2=3}^{\infty}\sum_{j_1=0}^{r_1}\sum_{j_2=0}^{r_2}C_{j_1j_2}^{r_1r_2}Q_1^{j_1}Q_2^{j_2}P_1^{r_1-j_1}P_2^{r_2-j_2}, \tag{9.2}$$

where $A_0^{2,0}=C_2^{2,0}$, etc. The other A's are at least continuous functions of the time. The C's need not be constant, but, as was remarked above, there seems little point in transforming from one time-dependent system to another. The type two generating function is

$$F_2(q_1,q_2,P_1,P_2,t)$$

$$=q_1P_1+q_2P_2+\sum_{r_1+r_2=3}^{\infty}\sum_{j_1=0}^{r_1}\sum_{j_2=0}^{r_2}B_{j_1j_2}^{r_1r_2}(t)$$

$$\times q_1^{j_1}q_2^{j_2}P_1^{r_1-j_1}P_2^{r_2-j_2}. \tag{9.3}$$

From the equation

$$\bar{H}(q_1,q_2,P_1,P_2,t)=H(q_1,q_2,P_1,P_2,t)+\frac{\partial F_2(q_1,q_2,P_1,P_2,t)}{\partial t} \tag{9.4}$$

we have

$$\begin{aligned}
&\sum_{j=0}^{2} C_j^{2,0}\left\{q_1+\sum\sum\sum (s_1-i_1)\,B_{i_1i_2}^{s_1s_2} q_1^{i_1} q_2^{i_2} P_1^{s_1-1-i_1} P_2^{s_2-i_2}\right\}^j P_1^{2-j}\\
&+\sum_{j=0}^{2} C_j^{0,2}\left\{q_2+\sum\sum\sum (s_2-i_2)\,B_{i_1i_2}^{s_1s_2} q_1^{i_1} q_2^{i_2} P_1^{s_1-i_1} P_2^{s_2-1-i_2}\right\}^j P_2^{2-j}\\
&+\sum\sum\sum C_{j_1j_2}^{r_1r_2}\left\{q_1+\sum\sum\sum (s_1-i_1)\,B_{i_1i_2}^{s_1s_2} q_1^{i_1} q_2^{i_2} P_1^{s_1-1-i_1} P_2^{s_2-i_2}\right\}^{j_1}\\
&\times\left\{q_2+\sum\sum\sum (u_2-k_2)\,B_{k_1k_2}^{u_1u_2} q_1^{k_1} q_2^{k_2} P_1^{u_1-k_1} P_2^{u_2-1-k_2}\right\}^{j_2} P_1^{r_1-j_1} P_2^{r_2-j_2}\\
&\quad=\sum_{j=0}^{2} A_j^{2,0} q_1^{2-j}\left\{P_1+\sum\sum\sum i_1 B_{i_1i_2}^{s_1s_2} q_1^{i_1-1} q_2^{i_2} P_1^{s_1-i_1} P_2^{s_2-i_2}\right\}^j\\
&\qquad+\sum_{j=0}^{2} A_j^{0,2} q_2^{2-j}\left[P_2+\sum\sum\sum i_2 B_{i_1i_2}^{s_1s_2} q_1^{i_1} q_2^{i_2-1} P_1^{s_1-i_1} P_2^{s_2-i_2}\right]^j\\
&\qquad+\sum\sum\sum A_{j_1j_2}^{r_1r_2} q_1^{r_1-j_1} q_2^{r_2-j_2}\left\{P_1+\sum\sum\sum i_1 B_{i_1i_2}^{s_1s_2} q_1^{i_1-1} q_2^{i_2} P_1^{s_1-i_1} P_2^{s_2-i_2}\right\}^{j_1}\\
&\qquad\times\left[P_2+\sum\sum\sum k_2 B_{k_1k_2}^{u_1u_2} q_1^{k_1} q_2^{k_2-1} P_1^{u_1-k_1} P_2^{u_2-k_2}\right]^{j_2}+\sum\sum\sum \dot{B}_{j_1j_2}^{r_1r_2} q_1^{j_1} q_2^{j_2} P_1^{r_1-j_1} P_2^{r_2-j_2}.
\end{aligned} \tag{9.5}$$

The triple summations are all of the form

$$\sum_{r_1+r_2=3}^{\infty}\sum_{j_1=0}^{r_1}\sum_{j_2=0}^{r_2}.$$

As in one-dimensional case, (8.5) may be separated into polynomials of degree m (say) which
(i) are linear in the $B_{j_1j_2}^{r_1r_2}$ for which $r_1+r_2=m$,
(ii) do not contain any B's for which $r_1+r_2>m$, and
(iii) may contain B's either linearly or nonlinearly for which $r_1+r_2<m$. For $m=2$ the terms cancel due to our choice of the earliest coefficients. For $m=3$, we have on separation of the coefficients of like powers, twenty linear differential equations of the type

$$\begin{aligned}
&\dot{B}_{j_1j_2}^{r_1r_2}+\{A_1^{2,0}j_1+A_1^{0,2}j_2\}B_{j_1j_2}^{r_1r_2}-\{C_1^{2,0}(r_1-j_1)\\
&\quad+C_1^{0,2}(r_2-j_2)\}B_{j_1j_2}^{r_1r_2}+2A_2^{2,0}(j_1+1)B_{j_1+1,j_2}^{r_1r_2}\\
&\quad+2A_2^{0,2}(j_2+1)B_{j_1,j_2+1}^{r_1r_2}-2C_2^{2,0}(r_1+1-j_1)B_{j_1-1,j_2}^{r_1r_2}\\
&\quad-2C_2^{0,2}(r_2+1-j_2)B_{j_1,j_2-1}^{r_1r_2}=C_{j_1j_2}^{r_1r_2}-A_{j_1j_2}^{r_1r_2}.
\end{aligned} \tag{9.6}$$

We have used the convention that any B's with $j_1(j_2)<0$ or $>r_1(r_2)$ are zero. For each B, $r_1+r_2=3$. This system, subject to the usual conditions on the A's, is integrable. For general m there will be $\frac{1}{6}(m+1)(m+2)(m+3)$ such equations.

We note that there is no problem concerning the commensurability of either A's or C's since the coefficient of any $\dot{B}$ is never zero.

10. DIRECT TRANSFORMATION APPROACH

We do not wish to repeat the detail of Secs. 5 and 6, but it is worthwhile noting that the direct transformation approach applies equally well for higher dimensional problems. We illustrate the point with the backwards method. Let

$$\begin{aligned}
&H(q_1,q_2,p_1,p_2,t)\\
&\quad=\tfrac{1}{2}(q_1^2+q_2^2+p_1^2+p_2^2)+\sum_3 A_{j_1j_2}^{r_1r_2}(t)q_1^{j_1}q_2^{j_2}p_1^{r_1-j_1}p_2^{r_2-j_2},
\end{aligned} \tag{10.1}$$

$$\bar{H}(Q_1,Q_2,P_1,P_2,)=\tfrac{1}{2}(Q_1^2+Q_2^2+P_1^2+P_2^2), \tag{10.2}$$

$$Q_1=q_1+\sum_2\sum\sum\sum B_{j_1j_2}^{r_1r_2}(t)q_1^{j_1}q_2^{j_2}p_1^{r_1-j_1}p_2^{r_2-j_2}, \tag{10.3}$$

$$Q_2=q_2+\sum_2\sum\sum\sum C_{j_1j_2}^{r_1r_2}(t)q_1^{j_1}q_2^{j_2}p_1^{r_1-j_1}p_2^{r_2-j_2}, \tag{10.4}$$

$$P_1=p_1+\sum_2\sum\sum\sum D_{j_1j_2}^{r_1r_2}(t)q_1^{j_1}q_2^{j_2}p_1^{r_1-j_1}p_2^{r_2-j_2}, \tag{10.5}$$

$$P_2=p_2+\sum_2\sum\sum\sum E_{j_1j_2}^{r_1r_2}q_1^{j_1}q_2^{j_2}p_1^{r_1-j_1}p_2^{r_2-j_2}, \tag{10.6}$$

where $\Sigma_3\Sigma\Sigma$ is

$$\sum_{r_1+r_2=3}^{\infty}\sum_{j_1=0}^{r_1}\sum_{j_2=0}^{r_2}$$

and $\Sigma_2\Sigma\Sigma$ starts with $r_1+r_2=2$.

Applying the standard criterion that the description of the motion must be equivalent in either coordinate system, we find that the transformation coefficients satisfy the system of equations

$$\begin{aligned}\dot{B}^{m_1m_2}_{k_1k_2}&+(k_1+1)\,B^{m_1m_2}_{k_1+1,k_2}+(k_2+1)\,B^{m_1m_2}_{k_1,k_2+1}\\&-(m_1+1-k_1)\,B^{m_1m_2}_{k_1-1,k_2}\\&-(m_2+1-k_2)\,B^{m_1m_2}_{k_1,k_2-1}-D^{m_1m_2}_{k_1k_2}\\&=(m_1+1-k_1)\,A^{m_1+1,m_2}_{k_1k_2}+\sum_1(j_1s_1-i_1r_1)\\&\times B^{r_1r_2}_{j_1j_2}A^{s_1s_2}_{i_1i_2}+\sum_2(j_2s_2-i_2r_2)\,B^{r_1r_2}_{j_1j_2}A^{s_1s_2}_{i_1i_2},\end{aligned}\tag{10.7}$$

$$\begin{aligned}\dot{D}^{m_1m_2}_{k_1k_2}&+(k_1+1)\,D^{m_1m_2}_{k_1+1,k_2}+(k_2+1)\,D^{m_1m_2}_{k_1k_2+1}\\&-(m_1+1-k_1)\,D^{m_1m_2}_{k_1-1,k_2}\\&-(m_2+1-k_2)D^{m_1m_2}_{k_1,k_2-1}+B^{m_1m_2}_{k_1k_2}\\&=-(k_1+1)\,A^{m_1+1,m_2}_{k_1+1,k_2}+\sum_2(j_1s_1-i_1r_1)\,B^{r_1r_2}_{j_1j_2}A^{s_1s_2}_{i_1i_2}\\&+\sum_2(j_2s_2-i_2r_2)\,B^{r_1r_2}_{j_1j_2}A^{s_1s_2}_{i_1i_2},\end{aligned}\tag{10.8}$$

together with similar equations for the C's and E's. In Σ_1, i_1+j_1 ranges to k_1+1, i_2+j_2, to k_2, r_1+s_1 to m_1+2 and r_2+s_2 to m_2. In Σ_2, the limits are reversed. The comparative simplicity of Eqs. (10.7) and (10.8) is due to the simplicity of $\bar{H}$ and use of the backwards approach. The forward approach yields a more complicated nonhomogeneous term. If $m_1+m_2=m$, the number of equations for each value of m is $\frac{2}{3}(m-3)(m^2+9m+2)$. The number of arbitrary constants is reduced by the six Poisson Bracket conditions

$$\begin{aligned}&[Q_1,P_1]=1,\quad [Q_1,Q_2]=0,\quad [Q_1,P_2]=0,\\&[P_1,Q_2]=0,\quad [P_1,P_2]=0,\quad [Q_2,P_2]=1.\end{aligned}\tag{10.9}$$

11. INTEGRALS OF THE MOTION

From the examples of two-dimensional Hamiltonians considered in the previous two sections, we see that the structure of the differential equations determining the coefficients of the transformations is not significantly different from those for the one-dimensional problem. We assert that this will be the case for the general n-dimensional problem.

We are able to establish the formal existence of integrals of the motion by choosing

$$\bar{H}(\mathbf{Q},\mathbf{P})=\tfrac{1}{2}\sum_{i=1}^{n}(Q_i^2+P_i^2).\tag{11.1}$$

It is well-known that $\bar{H}$ possess n^2-1 constants of the motion linearly independent of $\bar{H}$. These constants may be written in compact form as an invariant matrix (cf. Leach[9])

$$I=\begin{bmatrix}\mathbf{Q}\\ \mathbf{P}\end{bmatrix}[\mathbf{Q}^T,\mathbf{P}^T]+J\begin{bmatrix}\mathbf{Q}\\ \mathbf{P}\end{bmatrix}[\mathbf{Q}^T,\mathbf{P}^T]J^T,\tag{11.2}$$

where J is the $2n\times 2n$ symplectic matrix. The invariants have the form $Q_iQ_j+P_iP_j$ or $Q_iP_j-Q_jP_i$. In terms of the original coordinates $(\mathbf{q},\mathbf{p})$, the n^2 constants of the motion (including $\bar{H}$) will be invariants of the motion described by $H(\mathbf{q},\mathbf{p},t)$ provided that the transformation equations are convergent. If they are not, truncation may provide approximate integrals as was noted by Gustavson[13] for the time-independent problem. Finally, we note that, if H is independent of time, it is a constant of the motion not necessarily equal to $\bar{H}(\mathbf{q},\mathbf{p},t)$. In this case it would appear that there are n^2+1 constants of the motion although possibly H is some combination of the $I_{ij}(\mathbf{q},\mathbf{p},t)$.

12. COMMENT

We have seen that there are three ways of approaching the transformation from one polynomial Hamiltonian to another. We emphasize that the transformations are formal and that problems of convergence could cause considerable difficulty. In much of this work we took $\bar{H}$ to be the Hamiltonian of a simple harmonic oscillator to simplify the algebra. It may well be that, in a practical application, even if the transformation is convergent, the number of terms required for useful approximation is prohibitive. Better results may be obtained if the coefficients of $\bar{H}$ are chosen to be the mean values of the time-dependent coefficients of H. This is a distinct possibility if these coefficients are periodic functions of time.

The transformation method adopted depends upon our intention. A knowledge of the invariants may be more informative than a formal solution. It is possible that a knowledge of the generating function will be of use in the study of the corresponding problem in quantum mechanics. It has been shown (cf. Boon and Seligman,[16] Leach,[8] and Wolf[17]) that, for linear transformations, a solution of the Schrödinger equation.

$$H\psi=i\hbar\frac{\partial\psi}{\partial t}\tag{12.1}$$

may be obtained from

$$\bar{H}\bar{\psi}=i\hbar\frac{\partial\bar{\psi}}{\partial t}\tag{12.2}$$

by means of an integral transform. The kernel of the transform depends upon the generating function of the corresponding classical transformation. We suggest that there could be a similar result for nonlinear transformations. As this work on nonlinear transformations has shown, any calculation is complex. The problem is currently under investigation.

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Towards an invariant for the time-dependent anharmonic oscillator

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The Hamiltonians $H=(1/2)(p^2+q^2)+\lambda(t)q^3$ and $\bar{H}=(1/2)(P^2+Q^2)+Q^3$, where $\bar{\lambda}(t)=1$, are related by time-dependent polynomial canonical transformations. Formulas are constructed for the generating function $F_2(q,P,t)$ as well as for the direct relations between (Q,P) and (q,p). These formulas are expressed fairly concisely in terms of time integrals. The form is seen to be applicable to all polynomial transformations of time-dependent anharmonic oscillator systems.

1. INTRODUCTION

The motion of a charged particle in a time-dependent electromagnetic field is of interest in plasma physics. One of the simplest problems, that in which the field is axially symmetric, can be reduced to a discussion of the Hamiltonian (cf. Lewis[1])

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\omega^2(t)q^2, \tag{1.1}$$

where p and q are canonically conjugate coordinates. The Hamiltonian (1.1) and its invariant have received considerable attention elsewhere.[2,3]

More generally, there are terms of order higher than q^2 and the Hamiltonian is

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\omega^2(t)q^2+V(q,t), \tag{1.2}$$

where $V(q,t)$ is at least $O(q^3)$ as $q\to 0$. An adiabatic invariant series may be constructed for $H(1.2)$ using Kruskal's method.[4] However, no one has seen a way to apply his method to find an exact invariant, nor is the Hamiltonian amenable to treatment by the use of time-dependent linear canonical transformations.[3,5] However, the extra potential $V(q,t)$ can have an important bearing on the boundedness of the motion, hence the relevance to plasma problems.

It would be of interest to see if the explicit time dependence in $V(q,t)$ has any effect on the boundedness of the motion and for that purpose it would be of value if an invariant could be found for $H(1.2)$. In this paper we investigate one method of searching for such an invariant. A Hamiltonian which can have unbounded motion is one which contains a term in q^3 and so we shall discuss the Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\omega^2(t)q^2+\lambda(t)q^3 \tag{1.3}$$

[the sign of $\lambda(t)$ is immaterial]. It is not necessary to discuss as general a system as (1.3) since, under the linear canonical transformation

$$Q=\rho^{-1}q, \quad P=-\dot{\rho}q+\rho p, \tag{1.4}$$

where $\rho(t)$ is any solution of

$$\ddot{\rho}+\omega^2(t)\rho=\rho^{-3}, \tag{1.5}$$

(1.3) reduces to

$$H=\rho^{-2}(\tfrac{1}{2}P^2+\tfrac{1}{2}Q^2+\rho^5\lambda Q^3). \tag{1.6}$$

If the change of time variable

$$t'=\int\rho^{-2}(t)\,dt \tag{1.7}$$

is made, Hamilton's equations become

$$\frac{dQ}{dt'}=P, \quad \frac{dP}{dt'}=-(Q+3\rho^5\lambda Q^2). \tag{1.8}$$

Evidently the discussion of the problem of $H(1.3)$ is equivalent to that of the Hamiltonian

$$H=\tfrac{1}{2}(p^2+q^2)+\lambda(t)q^3. \tag{1.9}$$

It is this Hamiltonian which will be treated here.

The method used is that of polynomial time-dependent transformations.[5] Since such transformations must be considered as infinite series, difficulties with convergence are to be expected. Although, in theory,[6] there exists a transformation between any two Hamiltonians of the same number of degrees of freedom, series representations of such transformations need not be universally convergent (cf. Leach[7]). An *a priori* method to minimize the possibility of nonconvergence is to select a transformed Hamiltonian which as closely as possible resembles the original. To this end we assume that $\lambda(t)$ has a mean value of unity and, without specifying the nature of its time variation, presume that it is of limited variation about the mean value. Under these circumstances we take the transformed Hamiltonian to be

$$\bar{H}=\tfrac{1}{2}(P^2+Q^2)+Q^3. \tag{1.10}$$

The Hamiltonian (1.10) is time independent and, if it can be expressed in terms of the original coordinates q,p, will provide an invariant for $H(1.9)$. As a first step we show how to construct a generating function for the transformation from H to $\bar{H}$. The form of the generating function suggests a form for a direct transformation between (q,p) and (Q,P). This form is verified and the canonicity of the transformation is demonstrated. Despite the simplifications in expression which we have been able to make, the series remain infinite and formidable. It may be that in a truncated form they will be of some use.

2. THE GENERATING FUNCTION

Using a type two generating function $F_2(q,P,t)$ so that

$$p=\frac{\partial F_2}{\partial q}, \quad Q=\frac{\partial F_2}{\partial P}, \tag{2.1}$$

we write

$$F_2(q,P,t)=qP+\sum_{r=3}^{\infty}\sum_{j=0}^{r}A_j^r(t)\,q^jP^{r-j}. \tag{2.2}$$

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By making the leading term the identity transformation, in effect we are requiring that the A's vanish when $\lambda(t) = \bar{\lambda}(t) = 1$. Substituting (1.9), (1.10), and (2.2) into

$$\bar{H}(q, P, t) = H(q, P, t) + \frac{\partial F_2}{\partial t} \tag{2.3}$$

we obtain

$$\begin{aligned}\sum\{\dot{A}_j^r q^j p^{r-j} &+ jA_j^r q^{j-1} P^{r+1-j} - (r-j) A_j^r q^{j+1} P^{r-1-j}\} \\ &= (1-\lambda) q^3 + \tfrac{1}{2}\sum\sum\{(r-j)(s-i) q^{i+j} P^{r+s-2-i-j} \\ &\quad - ijq^{i+j-2} P^{r+s-1-j}\} A_j^r A_i^s + 3\sum (r-j) A_j^r q^{j+2} P^{r-1-j} \\ &\quad + 3\sum\sum (r-j)(s-i) A_j^r A_i^s q^{i+j+1} P^{r+s-2-i-j} \\ &\quad + \sum\sum\sum (r-j)(s-i)(u-k) A_j^r A_i^s A_k^u q^{i+j+k} P^{r+s+u-3-i-j-k},\end{aligned} \tag{2.4}$$

where each summation sign indicates summation as in (2.2). Equating coefficients of like powers, (2.4) is equivalent to

$$(ID + M)\,\mathbf{A}^r = \mathbf{v}^r \tag{2.5}$$

where $D = d/dt$, I is the $(r+1)\times(r+1)$ identity matrix, M an $(r+1)\times(r+1)$ matrix with the only nonzero elements being

$$M_{i+1,i} = -(r+1-i), \quad M_{i,i+1} = i, \tag{2.6}$$

$\mathbf{A}^r$ an $(r+1)$ vector formed from the A_j^r, $j = 0, r$ and $\mathbf{v}^r$ an $(r+1)$ vector whose elements come from the nonhomogeneous terms. In particular

$$\mathbf{v}^3 = (1-\lambda)\begin{bmatrix}0\\0\\0\\1\end{bmatrix}. \tag{2.7}$$

In general, $\mathbf{v}^r$ contains A's, but of index lower than r.

The coefficients A_j^r are found by the integration of the system of equations (2.5). A general solution for any r will contain $(r+1)$ arbitrary constants from the solution of the homogeneous part of (2.5). As these will feed into the equations for higher indices (through $\mathbf{v}$), they could represent a considerable complication in practice. Since we are dealing with a generating function, all of these arbitrary constants may be set at zero without affecting the canonicity of the transformation. Hence we only concern ourselves with the particular solution for the nonhomogeneous part of (2.5).

3. SOLUTION OF THE EQUATION $(ID + M)\,A^r = v^r$

The matrix M is skew-centrosymmetric, i.e.,

$$L^{-1}ML = -M, \tag{3.1}$$

where the elements of L are zero except for those along the secondary diagonal which are all unity. There exists a diagonal matrix D such that

$$D^{-1}MD = iN, \tag{3.2}$$

where N is symmetric. The nonzero elements of D are given by

$$d_{j+1,j+1} = i^j \binom{r}{j}^{1/2}, \quad j = 0, r \tag{3.3}$$

and those of N by

$$N_{j+1,j} = \{(r+1-j)\,j\}^{1/2} = N_{j,j+1}. \tag{3.4}$$

The matrix N is of known type[8] and its eigenvalues are $\pm r, \pm(r-2), \cdots, [\pm 1 \text{ or } 0]$. Hence the characteristic values of the system of differential equations (2.5) are $\pm ir, \pm i(r-2), \cdots, [\pm i \text{ or } 0]$.

The solution for the nonhomogeneous part of (2.5) may be determined by the method of variation of parameters. It is

$$\mathbf{A}^r = \mathbf{a}_0(t) + \sum_{j=1}^{r/2} [\mathbf{a}_{2j}(t)\cos 2jt + \mathbf{b}_{2j}(t)\sin 2jt] \tag{3.5}$$

for r even and

$$A^r = \sum_{j=0}^{(r-1)/2} [\mathbf{a}_{2j+1}(t)\cos(2j+1)\,t + \mathbf{b}_{2j+1}(t)\sin(2j+1)\,t] \tag{3.6}$$

for r odd. The vectors $\mathbf{a}_j$ and $\mathbf{b}_j$ satisfy the requirements

$$\begin{aligned} &M\mathbf{a}_0(t) = 0, \\ &M\mathbf{a}_j + j\mathbf{b}_j = 0, \quad j \neq 0, \\ &M\mathbf{b}_j - j\mathbf{a}_j = 0, \quad j \neq 0, \end{aligned} \tag{3.7}$$

and

$$\begin{aligned} &\dot{\mathbf{a}} + \sum(\dot{\mathbf{a}}_{2j}\cos 2jt + \dot{\mathbf{b}}_{2j}\sin 2jt) = \mathbf{v}^r, \quad r \text{ even} \\ &\sum[\dot{\mathbf{a}}_{2j+1}\cos(2j+1)\,t + \dot{\mathbf{b}}_{2j+1}\sin(2j+1)\,t] = \mathbf{v}^r, \quad r \text{ odd}. \end{aligned} \tag{3.8}$$

From (3.7) it is possible to write down recurrence relations for the elements of the $\mathbf{a}$'s and $\mathbf{b}$'s. In their general form they are not particularly simple and do not suggest an easy method for solving (3.8). However, the solutions of these equations for the first few values of r when substituted into (2.2) suggest that the generating function has the form

$$\begin{aligned} F_2(q, P, t) &= qP + \sum_{r=3}^{\infty}\sum_{j=0}^{r}\int_{t_0}^{t} v_j^r(t')[P\sin(t'-t) + q\cos(t'-t)]^j \\ &\quad \times\{P\cos(t'-t) - q\sin(t'-t)\}^{r-j}\,dt'. \end{aligned} \tag{3.9}$$

The value of t_0 is that value of t for which $\lambda(t) = 1$. We note that

$$\begin{aligned} \frac{\partial F_2}{\partial t} &= \sum_{r=3}^{\infty}\sum_{j=0}^{r} v_j^r(t)\,q^j P^{r-j} \\ &\quad + \sum_{r=3}^{\infty}\sum_{j=0}^{r}\int_{t_0}^{t} v_j^r(t')\{-j[P\sin(t'-t) + q\cos(t'-t)]^{j-1} \\ &\quad \times[P\cos(t'-t) - q\sin(t'-t)]^{r+1-j} \\ &\quad + (r-j)[P\sin(t'-t) + q\cos(t'-t)]^{j+1} \\ &\quad \times[P\cos(t'-t) - q\sin(t'-t)]^{r-1-j}\}\,dt'. \end{aligned} \tag{3.10}$$

It is merely a matter of routine algebra to show that this expression for $F_2(q, P, t)$ satisfies (2.3) and in fact (2.3) reduces to the definition of v_j^r given by (2.4) and (2.5).

4. DIRECT SOLUTION

Although it is informative to have the generating function of the transformation, it is more convenient to have (q, p) in terms of (Q, P, t) or vice versa. For the

purposes of this discussion we shall see how the invariant $\bar{H}(Q,P)$ may be written in terms of (q,p,t). We formally define (Q,P) in terms of (q,p,t) as

$$Q = q + \sum_{r=2}^{\infty} \sum_{j=0}^{r} B_j^r(t)\, q^j p^{r-j}, \tag{4.1}$$

$$P = p + \sum_{r=2}^{\infty} \sum_{j=0}^{r} C_j^r(t)\, q^j p^{r-j}. \tag{4.2}$$

Differential equations for the B's and C's are obtained by requiring that the time development of the system is equivalent in both (q,p) and (Q,P) coordinate systems. Proceeding in the usual way, we obtain the systems of equations for the coefficients B_j^r and C_j^r,

$$(ID + M)\,\mathbf{B}^r - \mathbf{C}^r = \mathbf{u}^r, \tag{4.3}$$

$$(ID + M)\,\mathbf{C}^r + \mathbf{B}^r = \mathbf{v}^r, \tag{4.4}$$

where the notation is consistent with that used in Secs. 2 and 3 above. Here $r = 2, 3, \cdots$. In particular, for $r = 2$, the nonhomogeneous terms are

$$\mathbf{u}^2 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{v}^2 = -3(1-\lambda)\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}. \tag{4.5}$$

Equations (4.3) and (4.4) may be combined into a single system

$$(ID + K)\,\mathbf{E}^r = \mathbf{w}^r, \tag{4.6}$$

where

$$K^r = \begin{bmatrix} M^r, & -I^r \\ I^r, & M^r \end{bmatrix}, \quad \mathbf{E}^r = \begin{bmatrix} \mathbf{B}^r \\ \mathbf{C}^r \end{bmatrix}, \quad \mathbf{w}^r = \begin{bmatrix} \mathbf{u}^r \\ \mathbf{v}^r \end{bmatrix}. \tag{4.7}$$

We note that, although we shall not discuss the form for p and q in terms of (Q,P,t), the equations have the same structure as given here.

5. SOLUTION OF THE EQUATION $(ID + K)\,E^r = 0$

In contrast with the generating function, the transformation equations (4.1) and (4.2) must satisfy the requirement that

$$[Q,P]_{PB(q,p)} = 1. \tag{5.1}$$

Consequently *ab initio* we cannot ignore the contribution of the homogeneous part of the solution of (4.6).

The eigenvalues of K are either pure imaginary or zero. This follows from the transformation

$$\begin{bmatrix} D^{-1} & 0 \\ 0 & D^{-1} \end{bmatrix} K \begin{bmatrix} D & 0 \\ 0 & D \end{bmatrix} = i \begin{bmatrix} N & iI \\ -iI & N \end{bmatrix} = iR \tag{5.2}$$

where D and N are defined by (3.3) and (3.4). As N is real symmetric, the matrix R in (5.2) is Hermitian and has real eigenvalues. Thus those of K are pure imaginary or zero. The values which the eigenvalues take may be found as follows. Suppose

$$R\mathbf{z} = \lambda\mathbf{z}, \tag{5.3}$$

where λ is real. Writing $\mathbf{z}^T = (\mathbf{x}^T, \mathbf{y}^T)$,

$$N\mathbf{x} + i\mathbf{y} = \lambda\mathbf{x}, \quad -i\mathbf{x} + N\mathbf{y} = \lambda\mathbf{y}. \tag{5.4}$$

Eliminating $\mathbf{y}$,

$$(N - \lambda I)^2\,\mathbf{x} - \mathbf{x} = 0$$

$$\Leftrightarrow [N - (\lambda - 1)I][N - (\lambda + 1)I]\,\mathbf{x} = 0 \tag{5.5}$$

which has nontrivial solutions provided

$$|N - (\lambda - 1)I| = 0 \quad \text{or} \quad |N - (\lambda + 1)I| = 0. \tag{5.6}$$

Hence the eigenvalues of K are λ_k given by

$$\lambda_k = i(\lambda_n \pm 1), \tag{5.7}$$

where the λ_N are the eigenvalues of N. For a given r, λ_K takes the values $\pm(r+1)\,i$, $\pm(r-1)\,i(2), \cdots$, $[\pm i \text{ or } 0](2)$ where the (2) indicates multiple eigenvalues.

The solution of the homogeneous part of (4.6) will be of the form

$$\begin{aligned} \mathbf{E}^{2r} = {} & \mathbf{a}_{2r+1}\sin(2r+1)\,t + \mathbf{c}_{2r+1}\cos(2r+1)\,t \\ & + \sum_{j=0}^{r-1}\{[\mathbf{a}_{2j+1} + \mathbf{b}_{2j+1}t]\sin(2j+1)\,t \\ & + [\mathbf{c}_{2j+1} + \mathbf{d}_{2j+1}t]\cos(2j+1)\,t\}, \end{aligned} \tag{5.8}$$

$$\begin{aligned} \mathbf{E}^{2r+1} = {} & \mathbf{a}_{2r+2}\sin(2r+2)\,t + \mathbf{c}_{2r+2}\cos(2r+2)\,t \\ & + \sum_{j=1}^{r}\{[\mathbf{a}_{2j} + \mathbf{b}_{2j}t]\sin_2 jt + [\mathbf{c}_{2j} + \mathbf{d}_{2j}t]\cos 2jt\} \\ & + \mathbf{c}_0 + \mathbf{d}_0 t, \end{aligned} \tag{5.9}$$

for r greater than or equal to one. The constant coefficient vectors satisfy the requirements that

$$\begin{aligned} & K^m\mathbf{a}_{m+1} - (m+1)\,\mathbf{c}_{m+1} = 0, \\ & (m+1)\,\mathbf{a}_{m+1} + K^m\mathbf{c}_{m+1} = 0, \end{aligned} \quad m = 2r, 2r+1, \tag{5.10}$$

$$\begin{aligned} & K\mathbf{b}_{j+1} - (j+1)\,\mathbf{d}_{j+1} = 0, \\ & (j+1)\,\mathbf{b}_{j+1} + K\mathbf{d}_{j+1} = 0, \end{aligned} \quad 0 < j < m, \tag{5.11}$$

$$\begin{aligned} & K\mathbf{a}_{j+1} - (j+1)\,\mathbf{c}_{j+1} = -\mathbf{b}_{j+1}, \\ & (j+1)\,\mathbf{a}_{j+1} + K\mathbf{c}_{j+1} = -\mathbf{d}_{j+1}, \end{aligned} \quad 0 < j < m, \tag{5.12}$$

$$\begin{aligned} & K^{2r+1}d_0 = 0, \\ & K^{2r+1}\mathbf{c}_0 = -\mathbf{d}_0. \end{aligned} \tag{5.13}$$

As the rank of the system (5.10) is two less than its order, $\mathbf{a}_{m+1}$ and $\mathbf{c}_{m+1}$ are describable in terms of two parameters. For (5.11), it is four less and each pair $\mathbf{b}_{j+1}$, $\mathbf{d}_{j+1}$ is describable in terms of four parameters. The same applies for the homogeneous part of (5.12). For (5.13), two parameters are required for $\mathbf{d}_0$ and two separate ones for the homogeneous part of $\mathbf{c}_0$. Thus for a given r, $4r+2$ parameters are required. However, the system (4.6) requires only $2r+2$ constants of integration. The cause of the discrepancy is found in the inconsistency of the sets of equations (5.12) and (5.13). A consistent solution is found only if all $\mathbf{b}$'s and $\mathbf{d}$'s are identically zero. By way of example we indicate the proof of this for the simplest case which is that of (5.13).

Suppressing the subscript, the first of (5.13) is

$$\begin{bmatrix} M & -I \\ I & M \end{bmatrix} \begin{bmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \end{bmatrix} = 0 \tag{5.14}$$

$$\Leftrightarrow (M^2 + I)\,\mathbf{d}_1 = 0, \quad \mathbf{d}_2 = M\mathbf{d}_1. \tag{5.15}$$

The nonzero elements of $M^2 + I$ are

$$\begin{aligned} & (M^2+I)_{j,j} = (1-2j)\,r + (2j^2 - 4j + 3), \\ & (M^2+I)_{j,j+2} = j(j+1), \qquad j = 1, 2, \cdots \\ & (M^2+I)_{j+2,j} = (r-j)(r+1-j). \end{aligned} \tag{5.16}$$

The equation relating the odd and even elements of $\mathbf{d}_1$ constitute separate sets and we may write

$$\mathbf{d}_1 = a\mathbf{e} + b\mathbf{f}, \tag{5.17}$$

where a and b are parameters and

$$e_{2j+2} = 0, \quad f_{2j+1} = 0, \quad j = 0, 1, \cdots. \tag{5.18}$$

Using (5.16) it is a simple matter to show that

$$\begin{aligned} e_{2j+1} &= (r-1)_{2j}/2^j j!, \\ f_{2j+2} &= (r-1)_{2j}/2^j j!, \end{aligned} \quad j = 0, 1, \cdots, \tag{5.19}$$

where

$$(r-1)_{2j} = \begin{cases} 1, & j = 0, \\ (r-1)(r-3)\cdots(r-1-2j), & j \neq 0. \end{cases} \tag{5.20}$$

Furthermore

$$\mathbf{d}_2 = M\mathbf{d}_1 = -a\mathbf{f} + b\mathbf{e} \tag{5.21}$$

so that

$$\mathbf{d} = a\begin{bmatrix} \mathbf{e} \\ -\mathbf{f} \end{bmatrix} + b\begin{bmatrix} \mathbf{f} \\ \mathbf{e} \end{bmatrix}. \tag{5.22}$$

Again suppressing the subscript, the second of (5.13) is

$$\begin{bmatrix} M & -I \\ I & M \end{bmatrix} \mathbf{c} = -a\begin{bmatrix} \mathbf{e} \\ \mathbf{f} \end{bmatrix} - b\begin{bmatrix} \mathbf{f} \\ \mathbf{e} \end{bmatrix}. \tag{5.23}$$

Operating from the left with the nonsingular matrix

$$\begin{bmatrix} I & -M \\ 0 & I \end{bmatrix}$$

(5.23) becomes

$$\begin{bmatrix} 0 & -M_2 - I \\ I & M \end{bmatrix} \mathbf{c} = -a\begin{bmatrix} 2\mathbf{e} \\ -\mathbf{f} \end{bmatrix} - b\begin{bmatrix} 2\mathbf{f} \\ \mathbf{e} \end{bmatrix}. \tag{5.24}$$

The matrix $M^2 + I$ has rank two less than its order. The first two rows may be reduced to zeros by elementary row operations. This is achieved by the nonsingular matrix U which has first and second rows,

$$1 \quad 0 \quad \frac{1}{r} \quad 0 \quad \frac{1\cdot 3}{r(r-2)} \quad 0 \quad \frac{1\cdot 3\cdot 5}{r(r-2)(r-4)} \cdots$$

$$0 \quad 1 \quad 0 \quad \frac{3}{r-2} \quad 0 \quad \frac{3\cdot 5}{(r-2)(r-4)} \quad 0 \quad \cdots.$$

The other elements are $U_{ij} = \delta_{ij}$, $i, j > 2$. The effect of U on the right side of (5.24) is to produce as first element

$$a\left(1 + \tfrac{1}{2}\frac{r-1}{r} + \frac{3\cdot 5}{2\cdot 4}\frac{(r-1)(r-3)}{r(r-2)}\cdots\right),$$

and as second element,

$$b\left(1 + \frac{3}{2}\frac{r-1}{r-2} + \frac{3\cdot 5}{2\cdot 4}\frac{(r-1)(r-3)}{r(r-2)}\cdots\right).$$

Since both terms in parentheses are positive, (5.24) is consistent only if $a = 0 = b$. The proof for the systems (5.12) is along similar lines.

Thus the solution of the homogeneous part of (4.6) is

$$\mathbf{E}^{2r} = \sum_{j=0}^{r}[\mathbf{a}_{2j+1}\sin(2j+1)t + \mathbf{c}_{2j+1}\cos(2j+1)t] \tag{5.25}$$

and

$$\mathbf{E}^{2r+1} = \sum_{j=1}^{r+1}(\mathbf{a}_{2j}\sin 2jt + \mathbf{c}_{2j}\cos 2jt) + \mathbf{c}_0 \tag{5.26}$$

for the even and odd cases respectively.

6. SOLUTION OF THE EQUATION $(ID + K)E^r = w^r$

Again the method of variation of parameters may be applied to the solution of the nonhomogeneous equation. From (5.25) and (5.26) the solution will have the form

$$\mathbf{E}^{2r} = \sum_{j=0}^{r}[\mathbf{a}_{2j+1}(t)\sin(2j+1)t + \mathbf{c}_{2j+1}(t)\cos(2j+1)t] \tag{6.1}$$

and

$$\mathbf{E}^{2r+1} = \sum_{j=1}^{r+1}[\mathbf{a}_{2j}(t)\sin 2jt + \mathbf{c}_{2j}(t)\cos 2jt] + \mathbf{c}_0(t) \tag{6.2}$$

for r even and odd respectively. The vector functions $\mathbf{a}_j(t)$ and $\mathbf{c}_j(t)$ satisfy the equations

$$\begin{aligned} &j\mathbf{a}_j(t) + K\mathbf{c}_j(t) = 0, \\ &K\mathbf{a}_j(t) - j\mathbf{c}_j(t) = 0, \end{aligned} \quad j = 1, \cdots \tag{6.3}$$

$$K\mathbf{c}_0(t) = 0, \tag{6.4}$$

$$\begin{aligned} &\sum[\dot{\mathbf{a}}_{2j+1}(t)\sin(2j+1)t + \dot{\mathbf{c}}_{2j+1}(t)\cos(2j+1)t] = \mathbf{w}^r, \ r \text{ even}, \\ &\sum[\dot{\mathbf{a}}_{2j}(t)\sin 2jt + \dot{\mathbf{c}}_{2j}(t)\cos 2jt] + \dot{\mathbf{c}}_0(t) = \mathbf{w}^r, \ r \text{ odd}. \end{aligned} \tag{6.5}$$

This system is very similar to that of (3.7) and the similarity suggests that an analogous form of solution exists. An examination of the first set (that for $r = 2$) indicates that the nonhomogeneous contribution to the series portion of (4.1) is

$$\begin{aligned} &\sum_{r=2}^{\infty}\sum_{j=0}^{r} B_j^r q^j p^{r-j} \\ &= \sum_{r=2}^{\infty}\sum_{j=0}^{r}\int_{t_0}^{t} dt'[u_j^r(t')\cos(t'-t) - v_j^r(t')\sin(t'-t)] \\ &\quad \times[p\sin(t'-t) + q\cos(t'-t)]^j[p\cos(t'-t) \\ &\quad - q\sin(t'-t)]^{r-j} \end{aligned} \tag{6.6}$$

and that of (4.2) is

$$\begin{aligned} &\sum_{r=2}^{\infty}\sum_{j=0}^{r} C_j^r q^j p^{r-j} \\ &= \sum_{r=2}^{\infty}\sum_{j=0}^{r}\int_{t_0}^{t} dt'[u_j^r(t)\sin(t'-t) + v_j^r(t')\cos(t'-t)] \\ &\quad \times[p\sin(t'-t) + q\cos(t'-t)]^j[p\cos(t'-t) \\ &\quad - q\sin(t'-t)]^{r-j}. \end{aligned} \tag{6.7}$$

That this is so may be verified directly by substitution into the original equations defining the B's and C's.

7. CANONICAL REQUIREMENT

The full solution of the transformation equations from (q, p) to (Q, P) coordinates is composed of the nonhomogeneous parts given in (6.6) and (6.7), a homogeneous contribution plus the identity. The homogeneous part contains arbitrary coefficients which feed

back into the u's and v's of higher order nonhomogeneous terms. We shall see that the transformation will still be canonical if these arbitrary coefficients are all set at zero, i.e., only the terms in (6.6) and (6.7), together with the identity, are necessary for the transformation.

The transformation is canonical provided

$$[Q,P]_{PB\,(q,p)}=1. \tag{7.1}$$

In an earlier paper[5] we showed that if a time-dependent transformation is canonical for some time $t=t_0$, then it is canonical for all time. Writing the transformation as

$$\begin{aligned} Q&=q+\sum_{r=2}^{\infty}\sum_{j=0}^{r}B_j^r q^j p^{r-j},\\ P&=p+\sum_{r=2}^{\infty}\sum_{j=0}^{r}C_j^r q^j p^{r-j}, \end{aligned} \tag{7.2}$$

where the summed terms are given by (6.6) and (6.7) respectively, it is immediately apparent that (7.1) is satisfied at $t=t_0$. Hence the transformation is canonical for all t and the homogeneous part may be ignored.

8. DISCUSSION

The expressions obtained here for both the generating function and the direct transformation equations are not simple, but at least they can be written down in a fairly concise form. It may be that some other method would yield a more closed solution, but, perhaps pessimistically, we doubt it. We note that the solutions given here are valid in form for any Hamiltonian

$$H=\tfrac{1}{2}(p^2+q^2)+V(q,t) \tag{8.1}$$

provided $V(q,t)$ has a Maclaurin expansion whose first term is cubic in q. In fact we may as well say $V(q,p,t)$. All that happens is that the vectors **u** and **v** have more complex defining relations.

The value of the transformations obtained here depends upon whether they converge. For time-independent problems, the convergence of similar series appears to be exceptional (cf. Moser[9] and the references cited therein). We have endeavored to minimize the possibility of divergence by using the mean value of H for $\bar{H}$. The work of Gustavson[10] encourages us to believe that truncated series may be of some use for sufficiently small values of $\bar{H}$ (i.e., the invariant). However, the form of the transformation equations suggests that if $\lambda(t)$ has a rational period, the transformation will blow up in time as at least one term in the transformation will be monotonically increasing in time.

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Percolation theory on multirooted directed graphs

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The multiroot connectedness $P_{u\mathbf{v}}$ of a directed graph G between the vertex u and the collection of vertices $\mathbf{v} = \{v_1,...,v_n\}$ is the probability that there are (directed) paths from u to each of the vertices v_i, $i = 1, ...,n$, when each edge and vertex has a given probability of being independently deleted. The properties of the coefficients in the expansion

$$P_{u\mathbf{v}}(G) = \Sigma_{A'\subseteq A}\vec{d}_{u\mathbf{v}}(G')\Pi_{a\in A'}p_a\,\Pi_{w\in V'}p_w,$$

where A and V are the arc and vertex sets of G respectively, $p_a(p_w)$ is the probability that an arc a (vertex w) is not deleted, and G' is the arc set A' together with its incident vertices V', are considered. The values of $\vec{d}_{u\mathbf{v}}(G)$ are characterized as follows: $\vec{d}_{u\mathbf{v}}(G)$ is shown to be nonzero if and only if G is coverable by paths and has no directed circuit. For this case $\vec{d}_{u\mathbf{v}}(G') = (-1)^{t_{u\mathbf{v}}+n} = (-1)^{\nu(G)}$, where $t_{u\mathbf{v}}$ is the maximal number of independent directed paths between u and the set $\mathbf{v}$, and $t_{u\mathbf{v}}$ is shown to be equal to $\nu(G)+n$, where $\nu(G)=|E|-|V|+1$ is the cyclomatic number of G.

INTRODUCTION

This paper generalizes the results in Ref. 1 on two rooted directed graphs to directed graphs with many roots. The weights associated with such graphs and their properties proved here are required in a forthcoming paper[2] on percolation theory in a gas. The result $\vec{d}_{u\mathbf{v}}(G) = (-1)^{\nu(G)}$ is also used in developing a relation between graphical expansions and renormalization for the percolation problem.[3]

Many of the proofs of the results given here follow those given in Ref. 1 and so they are omitted. Only the differences will be emphasized between the many-root and two-rooted situations.

A completely different proof of Theorem 5 on the directed–undirected d weight relation is given[4] in contrast to the inductive proof in Ref. 1.

Consider a graph G with input vertex u and output vertices $\mathbf{v}=\{v_1,...,v_n\}$ and suppose that a subset of the edges and vertices is deleted. G is sometimes denoted by $G_{u\mathbf{v}}$ if we wish to emphasize the root points of G. Let S_{u,v_i} be the set of all self-avoiding paths (following the arrows if G is directed) from u to v_i on G. For $s\in S_{u,v_i}$ define the indicator random variable

$$\gamma(s)=\begin{cases}1, & \text{if } s \text{ is open,}\\ 0, & \text{if } s \text{ is closed,}\end{cases}$$

in a given state of multilation of G. Now

$$\gamma_i \equiv \sum_{\phi\subset S_i\subseteq S_{u,v_i}} (-1)^{S_i+1}\prod_{s\in S_i}\gamma(s) \tag{2.1}$$

is one or zero according as there is at least one open path or no open path from u to v_i. The pair-connectedness is therefore given between u and v_i by

$$P_{u,v_i} = \langle\gamma_i\rangle = \sum_{\phi\subset S_i\subseteq S_{u,v_i}} (-1)^{|S_i|+1}\Big\langle\prod_{s\in S_i}\gamma(s)\Big\rangle.$$

Now let $g(S_i)$, $V(S_i)$, $E(S_i)$, $A(S_i)$ be the graph, the vertex set, the edge set, and the arc set obtained by taking the union of the paths in S_i. Thus if p_α is the probability that element α is not deleted, then

$$\Big\langle\prod_{s\in S_i}\gamma(s)\Big\rangle = \prod_{v\in V(S_i)}p_v\cdot\prod_{e\in E(S_i)}p_e,$$

since this is the probability that all the paths in S_i are open. The result may be expressed as a sum over subgraphs of G by grouping together all S_i for which $E(S_i)=E'$, and $g(S_i)=G'$; thus

$$P_{u,v_i} = \sum_{E'\subseteq E} d_{u,v_i}(G')\prod_{v\in V'}p_v\prod_{e\in E'}p_e,$$

where the "d weight" is given by

$$d_{u,v_i}(G') = \sum_{\substack{\phi\subset S_i\subseteq S_{u,v_i}\\ g(S_i)=G'}} (-1)^{|S_i|+1}.$$

For the directed case read A for E and $\vec{d}$ for d.

The extension to many outputs is now straightforward.

$P_{u,\mathbf{v}}$ = probability that there is a path from u to all of the output vertices

$$= \Big\langle\prod_{i=1}^{n}\gamma_i\Big\rangle = \sum_{E'\subseteq E} d_{u,\mathbf{v}}(g')\prod_{v\in V'}p_v\prod_{e\in E'}p_e \tag{2.2}$$

where

$$d_{u,\mathbf{v}}(G') = \prod_{i=1}^{n}\sum_{\phi\subset S_i\subseteq S_{u,v_i}} (-1)^{|S_i|+1}. \tag{2.3}$$
$$g(\overset{n}{\underset{i=1}{\cup}} S_i)=G'$$

If there does not exist $S=\overset{n}{\underset{i=1}{\cup}} S_i$ such that $g(S)=G'$, then $\vec{d}_{u\mathbf{v}}(G')=0$ from (2.3).

To establish a contraction–deletion rule for $\vec{d}_{u\mathbf{v}}$ weights let $p_a=1$, $p_w=1$ in (2.2). Then

$$\vec{\gamma}_{u\mathbf{v}}(G) = \sum_{A'\subseteq A}\vec{d}_{u\mathbf{v}}(G'), \tag{2.4}$$

where the connectedness indicator $\vec{\gamma}_{u\mathbf{v}}(G)$ is 1 if there are paths from u to each v_i of $G_{u\mathbf{v}}$ and zero otherwise.

Since the set of all subsets of the arc set A form a lattice, (2.4) may be inverted[2] to give

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$$\vec{d}_{uv}(G)=\sum_{A'\subseteq A}(-1)^{|A\setminus A'|}\vec{\gamma}_{uv}(G') \ . \tag{2.5}$$

Now consider a particular arc $a\in A$ and divide the sum according as $a\in A'$ and $a\notin A'$. We get

$$\vec{d}_{uv}\sum_{\substack{A'\subseteq A\\ a\in A'}}(-1)^{|A\setminus A'|}\vec{\gamma}_{uv}(G')+\sum_{\substack{A'\subseteq A\\ a\notin A'}}(-1)^{|A\setminus A'|}\vec{\gamma}_{uv}(G'). \tag{2.6}$$

Let G^{γ} be the graph G contracted along the arc a; that is, G^{γ} is the graph $G\setminus\{a\}$ with the adjacent vertices of a identified. Also we define G^{δ} to be the graph G with arc a deleted. If G' is a subgraph of G, we define G'^{γ} to be the graph with the arc and vertex set of G' with arc a contracted, and G'^{δ} to be G' less the arc a.

Thus if we ensure the arc a is oriented out of u it is clear that $\vec{\gamma}_{uv}(G')=\vec{\gamma}_{uv}(G'^{\gamma})$ when $a\in A'$. This true even if the arc a has a root v_i as an adjacent vertex if we assume that when $u=v_i$, then u and v_i are connected. Furthermore in the second summation G' does not contain the arc a and so $\vec{\gamma}_{uv}(G')=\vec{\gamma}_{uv}(G^{\delta})$ since $G'=G^{\delta}$.

It follows that

$$\vec{d}_{uv}(G)=\vec{d}_{uv}(G^{\gamma})-\vec{d}_{uv}(G^{\delta}) \tag{2.7}$$

subject to a being oriented out of u.

Remark: When $u=v_i$ on contraction, $\vec{d}_{uv}(G^{\gamma})=\vec{d}_{uv'}(G^{\gamma})$, where $v'=v\setminus\{v_i\}$ if we define $\vec{\gamma}_{uu}(G^{\gamma})=1$.

2. STATEMENT OF RESULTS

As stated above the d weight of a graph which is not coverable is zero. The following theorems apply to the d weight of a coverable multirooted graph G.

Theorem 1: The directed d weight is ± 1 or 0.

Theorem 2: The directed d weight is zero if an only if G has a circuit.

Definition: A collection $\mathscr{C}=\{\pi_i|i=1,...,n\}$ of (directed) paths on a coverable directed graph G_{uv} is said to be independent if the matrix $M=[m_{ij}]$ has maximal row rank where $\pi_i=\sum_{j=1}^{l}m_{ij}a_j$, $\pi_i\in\mathscr{C}$, and $a_j|j=1,...,l$ is the collection of arcs in G_{uv}, and $m_{ij}\in\mathbb{Q}$. Such a collection $\mathscr{C}$ is said to be *maximal* if every path not in $\mathscr{C}$ is dependent on the elements of $\mathscr{C}$. Obviously the number of paths in such a class is an invariant of G_{uv}. We will call such a set a maximal independent set (MIS) for G_{uv}.

Theorem 3: If the directed graph has no circuit, then

$$\vec{d}_{uv}(G)=(-1)^{t_{uv}+n}$$

where t_{uv} is the order of a MIS for G_{uv}

Theorem 4: For a directed graph G with no circuit $t_{uv}=\nu(G)+n$, where $\nu(G)=|E|-|V|+1$ is the cyclomatic number for G.

Note $\vec{d}_{uv}(G)=(-1)^{\nu(G)}$ follows from Theorems 3 and 4.

Theorem 5: The undirected d weight of G is equal to the sum of the directed $\vec{d}$ weights of G over all possible orientations of G.

3. Remarks and proofs of results

The basic graph which is the terminal stage of the reduction process using the contraction–deletion rule which was described in Sec. 1 is the multiroot parallel graph: Every arc is adjacent to the input root point u and one of the output root points of v.

Proof of Theorem 1: First of all is it assumed that v, the set of output root points, contains sinks and at each stage in the reduction process the arc $[u,w]$ is chosen so that w is not a sink. The theorem then follows since the reduction process ensures that $\vec{d}_{uv}(G)=0$ *or* $|\vec{d}_{uv}(G)|=|\vec{d}_{uv'}(G')|$, where G' is a parallel graph with input u and output $v_k=\{v_{i_1},...,v_{i_k}\}$, the set of sinks in v. Therefore, $|\vec{d}_{uv}(G)|=\pm 1$ or 0.

For the purposes of calculation the assumption that $v_k\neq\emptyset$ is no real restriction because $\vec{d}_{uv}(G)=\vec{d}_{uv}(G_e)$ where G_e is the union of G with a single arc b attached to a root point v_i where v_i is replaced by v_e as the root point, and b is oriented from v_i to v_e.

It can be further seen that if G does not have any root points which are sinks then there is a directed circuit in G and so the first part of Theorem 2 applies which will result in $\vec{d}_{uv}(G)=0$.

Proof of Theorem 2: This proof follows the corresponding Theorem 3 in Ref. 1. The only essential difference is that if $[u,w]$, the arc upon which the contraction–deletion rule is applied, is such that w is a root, then

$$\{\pi_i'\}_1^r\cup\{\pi_i\}_1^s\cup\{\pi_i\circ\pi_j''\}_1^{s,t}$$

is a covering for G^{δ}.

Proof of Theorem 3: As in the proof of the first part of Theorem 2 ($\leftrightarrow$), we can apply the contraction–deletion to an arc a of G with vertices u and w and contain two cases:

(1) $\vec{d}_{uv}(G^{\gamma})=\vec{d}_{uv}(G)$, G^{γ} has no circuit,

(2) $\vec{d}_{uv}(G^{\delta})=-\vec{d}_{uv}(G)$, G^{δ} has no circuit,

where G^{γ} and G^{δ} are both coverable. When w is not a root point it is easily shown, as in Theorem 4,[1] that number of independent paths in G and G^{γ} are equal and differs from the number independent paths in G^{δ} by one.

If w is a root point say v_1, then there is a natural one–one correspondence between paths on G^{γ} and the set of paths on G not including the root path π consisting of the (contracted) arc a between u and v_1.

A maximal independent set of contracted paths $\mathscr{C}^{\gamma}$ on G^{γ} gives rise to an independent set $\mathscr{C}'$ on G using the 1–1 correspondence.

We claim that $\mathscr{C}=\mathscr{C}'\cup\{\pi\}$ is a maximal independent set for paths on G. The set $\mathscr{C}$ is independent because if $\pi=\Sigma_{i=1}^{n}\alpha_i\pi_i$, $\pi_i\in\mathscr{C}'$, $\alpha_i\in\mathbb{Q}$, then on the contracted graph G^{γ}, $\pi^{\gamma}=\Sigma_{i=1}^{n}\alpha_i\pi_i^{\gamma}$; but $\pi^{\gamma}=\mathbf{0}$, the π_i^{γ} are independent, and not all the α_i's are zero since $\pi\neq\mathbf{0}$, so we have a contradiction.

To show that $\mathscr{C}$ is maximal on G suppose there exists a path $\pi_0(\neq\pi)$ such that $\mathscr{C}\cup\{\pi_0\}$ is independent. However the contracted path π_0^γ must be a linear sum of the MIS for G^γ, that is

$$\pi_0^\gamma=\sum_{i=1}^{n}\alpha_i\pi_i^\gamma,\ \pi_i^\gamma\in C^\gamma,\ \alpha_i\in\mathbb{Q},\ \alpha_i\neq 0,\ \text{for some } i.$$

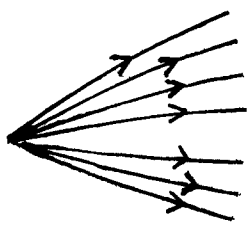
For the cases $a\in\pi_0$, $a\notin\pi_0$ the coefficients α_i at the vertex w sum to 1 and 0, respectively, therefore

$$\pi_0=\sum_{i=1}^{n}\alpha_i\pi_i,\ \text{and so we have a contradiction.}$$

Thus when w is a root point the number of independent paths in G and G^γ differ by one.

The other cases follow as in Theorem 4.[1]

Repeated application of the contraction–deletion process results in a parallel graph H of the following type:



Note there will in general be only k of the original n roots, say $v'=\{v_1,...,v_k\}$, the set of sinks which is nonempty by the no-circuit property. Moreover $d_{uv}(H)=+1=(-1)^{t_{uv_k}+k}$, where $t_{uv_k}(=k)$ is the number of independent paths in H.

Furthermore in the reduction process from G to H the number of independent paths has changed by one: (a) for every reduction by deletion, (b) for every reduction by contraction of a root point.

Therefore, the total change in the number of independent paths $t_{uv}-t_{uv_k}=(n-k)+\#$ of deletions

and hence the number of sign changes in the $\vec{d}$ weight for the sequence of graphs from G to H is

$$t_{uv}-t_{uv_k}-(n-k),$$

since $n-k$ is the number of roots contracted.

Therefore,

$$\vec{d}_{uv}(G)=(-1)^{t_{uv_k}+k+t_{uv}-t_{uv_k}-(n-k)}$$

$$=(-1)^{t_{uv}+n},$$

where t_{uv} is the number of independent paths in G.

Proof of Theorem 4: Let $\Pi=\{\pi_i|i=1,...,I\}$ be a MIS for G. The generalization required here is that G_0 be a subgraph of G consisting of a subset $\{\pi_i|i=1,...,n\}$ of Π covering all the root points. We can always take G_0 to be a tree.

The order of a MIS for G_0 is $n=|v|$. Moreover it is easy to check that $\vec{d}_{uv}(G)=+1$. Let $\rho_1,...,\rho_k$ be paths in Π which are not in G_0.

Define a sequence of subgraphs $G_i=G_0\cup\{\cup_{j=1}^{i}\rho_j\}$. For the sequence G_i define $\mu(G_i)=|E_i|-|V_i|+1+n$. We note $\mu(G_0)=n$ which is the number of paths in a MIS for G_0.

The argument now closely follows Theorem 5[1] and we obtain $\mu(G)=\mu(G_k)=t_{uv}$. Now $\mu(G)=\nu(G)+n$, where $\nu(G)$ is the cyclomatic number.[5] Therefore,

$$\vec{d}_{uv}(G)=(-1)^{t_{uv}+n}=(-1)^{\nu(G)+n+n}=(-1)^{\nu(G)}.$$

Proof of Theorem 5: Let G be an undirected graph and $\mathscr{D}(G)$ be the set of graphs obtained by directing G in all possible ways. Now consider the paths on G as directed from u to v_i. Any subset of S_i which covers G either covers some $g\in\mathscr{D}(G)$ or $g(S_i)$ has at least one loop of length 2. Let $\mathscr{L}(G)$ be the set of graphs obtained from g by directing it in all possible ways and replacing at least one edge by a loop of length 2. Thus

$$d_{uv_i}(G)=\sum_{\vec{g}\in\mathscr{L}(G)}\ \sum_{\substack{\phi\subset S_i\subseteq S_{uv_i}\\ g(S_i)=\vec{g}}}(-1)^{|S_i|+1}$$

$$\times\sum_{\vec{g}\in\mathscr{L}(G)}\ \sum_{\substack{\phi\subset S_i\subseteq S_{uv_i}\\ g(S_i)=\vec{g}}}(-1)^{|S_i|+1}. \tag{4.1}$$

But for $\vec{g}\in\mathscr{L}(G)$,

$$\sum_{\substack{\phi\subset S_i\subseteq S_{uv_i}\\ g(S_i)=\vec{g}}}(-1)^{|S_i|+1}=0 \tag{4.2}$$

since it is the $\vec{d}$ weight of a directed graph with a loop and the result follows by substituting (4.1) with condition (4.2) in (2.3).

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Predictive relativistic mechanics

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We integrate the partial differential equations on the accelerations in predictive relativistic mechanics by means of integro-functional equations. We investigate some problems concerning the Hamiltonian formulation of this mechanics: Poisson brackets of position variables of each particle, Hamilton–Jacobi equations, and Hamiltonian formulation of the separation of the external and internal motions.

INTRODUCTION

Contrary to the mechanics of particles interacting through propagating fields, a description involving an infinite number of degrees of freedom, PRM (predictive relativistic mechanics) restricts itself to systems of second-order differential equations; this means that initial positions and velocities suffice to predict the motion, hence the predictive qualificative to this mechanics. This is completed by the requirement of invariance under the Poincaré group; this means that, given a set of integral curves of the system in a Lorentz frame, the equation of these curves has the same form in any other Lorentz frame; or, in other words, the corresponding accelerations are the same functions of positions and velocities in any Lorentz frame.

Finite predictivity and relativistic invariance imply very restrictive nonlinear conditions on the accelerations; in Sec. 1A we give them for a formalism in which the predictiveness is manifest, the given conditions then guaranteeing the invariance, and in Sec. 1B for a formalism in which the invariance is made manifest at the start by the use of 4-vectors, the conditions then guaranteeing the predictiveness.

Predictivity and invariance are two general requirements, and an ingredient is necessary to characterize a specific interaction. We thus call upon field theories and use relations such as the Liénard–Wiechert formulae for electromagnetism as boundary conditions to integrate the equations given in Sec. 1B. This leads to coupled integrofunctional equations which can be solved step by step by developing accelerations in power series of a parameter such as a coupling constant. An approximation then characterizes the first term of the series, subsequent terms bringing in successive corrections to this first approximation. The explicit method of Sec. 2A uses the uniform motion approximation and yields accelerations explicitly in terms of positions and velocities. The semi-implicit method of Sec. 2B uses the relativistic uniformly accelerated motion, and yields accelerations in terms of positions, velocities, and accelerations themselves, thus implying a final inversion to get the accelerations in explicit form. This last approximation being closer to real motion, this method yields better results as illustrated on two particular examples.

Section 3A recalls the Hamiltonian formulation of such a mechanics, in which all symmetry transformations—predictivity and special relativity—are canonically represented.

It is well known that in such a frame particle positions cannot be canonical variables. However, we show in Sec. 3B that Poisson brackets of position variables of each particle (not between different ones) vanish up to first order in the coupling constant as a direct consequence of the existence in field theories of one variational principle per particle, respectively admitting the position variables of each particle as private Lagrangian coordinates.

The Hamiltonian formulation of Sec. 3A naturally exhibits one Hamiltonian per particle. In Sec. 3C we construct first the corresponding Lagrangians, and then one common variational principle with a variation procedure of its own. The concept of canonical transformation leads to the theory of Hamilton–Jacobi (HJ) whose principal feature is the existence of as many equations on the same generating function as particles; these HJ equations offer an interesting prelude to quantum mechanics.

At last, in Sec. 3D, we define the Hamiltonian formulation of the separation of external and internal motions. This begins by the introduction of the external variables: the total linear momentum of the system, and a conjugate, the center of spin, generalizing at the relativistic level the characteristic properties of the Newtonian center of mass. Then we find the equations to integrate to obtain the internal canonical variables.

1. EQUATIONS ON THE ACCELERATIONS IN PREDICTIVE RELATIVISTIC MECHANICS

A. Manifestly predictive formalism

PRM contemplates a fixed number of n point particles whose evolution is governed by a system of second-order differential equations[1]

$$\frac{dx^i_a}{dt}=v^i_a, \quad \frac{dv^i_a}{dt}=a^i_a(x^j_b,v^k_c;t) \tag{1.1}$$

which is invariant under the ten-parameter Poincaré group. Let us define precisely this invariance[2]: Let

$$x^i_a=\varphi^i_a(\overset{j}{x}_{0b},\overset{k}{v}_{0c};t), \tag{1.2a}$$

with

$$\underset{0}{x}{}^i_a=\varphi^i_a(\underset{0}{x}{}^j_b,\underset{0}{v}{}^k_c;0) \tag{1.2b}$$

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be the equations of n integral curves of (1.1) and consider the following n parametrized curves in Minkowski space M_4:

$$x^i_a = \varphi^i_a(x^j_{0b}, v^k_{0c}; t), \quad x^0_a = t. \tag{1.3}$$

Invariance under the Poincaré group means, using the active point of view, that for any transformation of this group whose ten parameters are denoted by $\Lambda^I, I=1,2,\ldots,10$, there exists functions f^i_a and g^i_a

$$x'^i_{0a} = f^i_a(x^j_{0b}, v^k_{0c}; \Lambda^I), \quad v'^i_{0a} = g^i_a(x^j_{0b}, v^k_{0c}; \Lambda^I) \tag{1.4}$$

such that the equations of the transformed curves use the same φ^i_a

$$x'^i_a = \varphi^i_a(x'^j_{0b}, v'^k_{0c}; t), \quad x'^0_a = t. \tag{1.5}$$

This requires

$$\frac{\partial a^i_a}{\partial t} = 0, \tag{1.6a}$$

$$\epsilon_b \frac{\partial a^i_a}{\partial x^j_b} = 0, \tag{1.6b}$$

$$\epsilon^l{}_{kj}\left(x^k_a \frac{\partial}{\partial x^l_a} + v^k_a \frac{\partial}{\partial v^l_a}\right) a^i_b = \epsilon^i{}_{kj} a^k_b, \tag{1.6c}$$

$$\left[(x_{aj} - x_{bj}) v^l_a \frac{\partial}{\partial x^l_a} + (v^l_a v_{aj} - \epsilon_a \delta^l_j + (x_{aj} - x_{bj}) a^l_a) \frac{\partial}{\partial v^l_a}\right] a^i_b = 2 v_{bj} a^i_b + v^i_b a_{bj}, \tag{1.6d}$$

where $\epsilon_a \equiv 1$, δ^i_j is the Kronecker symbol, and ϵ_{ijk} is the Levi-Civitta symbol.

These conditions were given for the first time independently by Currie[3] and Hill[4] as necessary conditions, and Bel[2] proved their sufficiency.

Consider the following ten vector fields:

$$\begin{aligned}
\mathbf{H} &= -v^i_a \frac{\partial}{\partial x^i_a} - a^i_a \frac{\partial}{\partial v^i_a}, \\
\mathbf{P} &= -\epsilon_a \frac{\partial}{\partial x^i_a}, \\
\dot{\mathbf{J}}_k &= \epsilon_k{}^i{}_j \left(x^j_a \frac{\partial}{\partial x^i_a} + v^j_a \frac{\partial}{\partial v^i_a}\right), \\
\mathbf{K}_j &= -x_{aj} v^i_a \frac{\partial}{\partial x^i_a} + (\epsilon_a \delta^i_j - v^i_a v_{aj} - x_{aj} a^i_a) \frac{\partial}{\partial v^i_a}.
\end{aligned} \tag{1.7}$$

Conditions (1.6b, c, d) are equivalent to requiring that the preceding generators satisfy the usual commutation rules characteristic of the Poincaré Lie algebra

$$\begin{aligned}
&[\mathbf{P}_i, \mathbf{H}] = 0, \quad [\dot{\mathbf{J}}_i, \mathbf{H}] = 0, \quad [\mathbf{K}_i, \mathbf{H}] = \mathbf{P}_i, \\
&[\mathbf{P}_i, \mathbf{P}_j] = 0, \quad [\dot{\mathbf{J}}_i, \mathbf{P}_j] = \epsilon_{ij}{}^k \mathbf{P}_k, \\
&[\mathbf{K}_i, \mathbf{P}_j] = \delta_{ij} \mathbf{H}, \quad [\dot{\mathbf{J}}_i, \dot{\mathbf{J}}_j] = \epsilon_{ij}{}^k \dot{\mathbf{J}}_k, \\
&[\mathbf{K}_i, \dot{\mathbf{J}}_j] = \epsilon_{ij}{}^k \mathbf{K}_k, \quad [\mathbf{K}_i, \mathbf{K}_j] = -\epsilon_{ij}{}^k \dot{\mathbf{J}}_k.
\end{aligned} \tag{1.8}$$

They are then called the generators of the realization of the Poincaré group induced on the phase space of the system (positions and velocities).

In this formalism, predictivity is manifest in Eq. (1.1), since initial positions and velocities suffice to predict the motion. Invariance under the Poincaré group is guaranteed by Eqs. (1.6).

B. Manifestly invariant formalism

Consider the following system of second-order differential equations on M_4:

$$\frac{dx^\alpha_a}{d\lambda} = \pi^\alpha_a, \quad \frac{d\pi^\alpha_a}{d\lambda} = \theta^\alpha_a(x^\beta_b, \pi^\gamma_c) \tag{1.9}$$

and require that the family of its integral curves be the same as that of (1.1). There is no unique way to do this. One way[5] adopts the $\pi^\alpha_a \pi_{a\alpha}$ as first integrals, thus offering the possibility of identifying them with minus the square of the masses m_a. This implies the following conditions[6]:

$$\pi^\alpha_a \theta_{a\alpha} = 0, \tag{1.10a}$$

$$\epsilon_b \frac{\partial \theta^\alpha_a}{\partial x^\beta_b} = 0, \tag{1.10b}$$

$$(\delta^\rho_\lambda \eta_{\mu\sigma} - \delta^\rho_\mu \eta_{\lambda\sigma})\left(x^\sigma_b \frac{\partial}{\partial x^\rho_b} + \pi^\sigma_b \frac{\partial}{\partial \pi^\rho_b}\right)\theta^\alpha_a = \delta^\alpha_\lambda \theta_{a\mu} - \delta^\alpha_\mu \theta_{a\lambda}, \tag{1.10c}$$

$$\left(\pi^{a\alpha} \frac{\partial}{\partial x^\alpha_a} + \theta^{a\alpha} \frac{\partial}{\partial \pi^\alpha_a}\right)\theta^\beta_{a'} = 0. \tag{1.10d}$$

These conditions are equivalent to saying that the following $10+n$ field vectors:

$$\begin{aligned}
\mathbf{P}_\lambda &= \epsilon_b \frac{\partial}{\partial x^\lambda_b}, \\
\dot{\mathbf{J}}_{\lambda\mu} &= (\delta^\rho_\lambda \eta_{\mu\sigma} - \delta^\rho_\mu \eta_{\lambda\sigma}) \times \left(x^\sigma_b \frac{\partial}{\partial x^\rho_b} + \pi^\sigma_b \frac{\partial}{\partial \pi^\rho_b}\right), \\
\mathbf{H}_a &= \pi^{a\lambda} \frac{\partial}{\partial x^\lambda_a} + \theta^{a\lambda} \frac{\partial}{\partial \pi^\lambda_a},
\end{aligned} \tag{1.11}$$

called the generators of the complete symmetry group, satisfy in addition to commutation rules characteristic of the Poincaré Lie algebra (trivially)

$$\begin{aligned}
&[\mathbf{P}_\lambda, \mathbf{P}_\mu] = 0, \\
&[\dot{\mathbf{J}}_{\mu\nu}, \dot{\mathbf{J}}_{\lambda\sigma}] = \eta_{\mu\lambda} \dot{\mathbf{J}}_{\nu\sigma} + \eta_{\nu\sigma} \dot{\mathbf{J}}_{\mu\lambda} - \eta_{\mu\sigma} \dot{\mathbf{J}}_{\nu\lambda} - \eta_{\nu\lambda} \dot{\mathbf{J}}_{\mu\sigma}, \\
&[\mathbf{P}_\lambda, \dot{\mathbf{J}}_{\mu\nu}] = \eta_{\lambda\nu} \mathbf{P}_\mu - \eta_{\lambda\mu} \mathbf{P}_\nu,
\end{aligned} \tag{1.12}$$

the following ones:

$$[\mathbf{H}_a,\mathbf{P}_\lambda]=0,\ [\mathbf{H}_a,\dot{\mathbf{J}}_{\lambda\mu}]=0,$$
$$[\mathbf{H}_a,\mathbf{H}_{a'}]=0,\ \mathscr{L}(\mathbf{H}_a)\pi_a^\alpha\pi_{a\alpha}=0. \tag{1.13}$$

One important consequence[5] of (1.10d) is that if

$$x_a^\alpha=\Phi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\lambda),\ \pi_a^\alpha=\Psi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\lambda), \tag{1.14a}$$

with

$$\overset{0}{x}{}_a^\alpha=\Phi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;0),\ \overset{0}{\pi}{}_a^\alpha=\Psi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;0) \tag{1.14b}$$

is the general integral of (1.9), then any element of it

$$\overset{0}{x'}{}_a^\alpha=\Phi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\overset{0}{\lambda}{}_a),\ \overset{0}{\pi'}{}_a^\alpha=\Psi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\overset{0}{\lambda}{}_a) \tag{1.15}$$

is a possible set of initial conditions for the same curves; moreover

$$x_a^\alpha=\Phi_a^\alpha(\overset{0}{x'}{}_b^\beta,\overset{0}{\pi'}{}_c^\gamma;\lambda-\overset{0}{\lambda}{}_a),$$
$$\pi_a^\alpha=\Psi_a^\alpha(\overset{0}{x'}{}_b^\beta,\overset{0}{\pi'}{}_c^\gamma;\lambda-\overset{0}{\lambda}{}_a). \tag{1.16}$$

Invariance of (1.9) under the Poincaré group is manifest in this formalism through (1.10b,c) which integrate immediately, and which say that the θ_a^α should be space–time translation and rotation invariant 4-vectorial functions of $x_a^\beta-x_{a'}^\beta$ and π_b^γ. Finite predictivity is seen through (1.10d).

Both the manifestly predictive and manifestly invariant formalisms are locally equivalent, and connection is biunivocally given by

$$a_a^i(x_b^j,v_c^k)=m_a^{-2}(1-v_a^2)(\delta_j^i-v_a^iv_{aj})\theta^j{}_a \tag{1.17}$$

where, in $\theta^j{}_a$, we set

$$x^0{}_b=t,\ \pi^i{}_b=m_b v^i{}_b(1-v^2{}_b)^{-1/2},$$
$$\pi^0{}_b=m_b(1-v^2{}_b)^{-1/2},v^2{}_b\equiv v^i{}_b v_{bi}. \tag{1.18}$$

This shows that π_a^α is $m_a u_a^\alpha$, where u_a^α is the usual 4-velocity, and that λ can be interpreted as $m_a^{-1}\tau_a$, where τ_a is the usual proper time elapsed from the initial configuration to the present one.

The following system

$$\frac{dx_a^\alpha}{d\tau}=u_a^\alpha,\ \frac{du_a^\alpha}{d\tau}=A_a^\alpha(x_b^\beta,u_c^\gamma), \tag{1.19}$$

where $A_a^\alpha=m_a^{-2}\theta_a^\alpha(x_b^\beta,\pi_c^\gamma=m_c u_c^\gamma)$ has the same integral curves as (1.9). The predictivity conditions then read

$$\left(u^{a'\alpha}\frac{\partial}{\partial x_{a'}^\alpha}+A^{a'\alpha}\frac{\partial}{\partial u_{a'}^\alpha}\right)A_a^\beta=0. \tag{1.20}$$

Note at last that (1.9) can also be stated as

$$\frac{dx_a^\alpha}{d\lambda_b}=\delta_a^b\pi_b^\alpha,\ \frac{d\pi_a^\alpha}{d\lambda_b}=\delta_a^b\theta_b^\alpha(x_c^\beta,\pi_d^\gamma) \tag{1.21}$$

the general integral being

$$x_a^\alpha=\Phi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\lambda_a),\ \pi_a^\alpha=\Psi_a^\alpha(\overset{0}{x}{}_b^\beta,\overset{0}{\pi}{}_c^\gamma;\lambda_a). \tag{1.22}$$

The manifestly predictive formalism is more fundamental, while the manifestly invariant one is more convenient for calculations.

2. INTEGRATION OF THE EQUATIONS OF THE MANIFESTLY INVARIANT FORMALISM

A. Integration in explicit form[7]

Assume equations of motion of the form

$$\frac{d\pi_a^\alpha}{d\lambda_a}=\sum_{a'}\mu_{aa'}\theta^{*\alpha}_a(x_a^\beta-x_{a'}^{\beta\,\mathrm{ret}},\pi_a^\gamma,\pi_{a'}^{\delta\,\mathrm{ret}},\theta_{a'}^{\xi\,\mathrm{ret}})$$
$$+(1-\mu_{aa'})\theta^{*\alpha}_a(x_a^\beta-x_{a'}^{\beta\,\mathrm{adv}},\pi_a^\gamma,\pi_{a'}^{\delta\,\mathrm{adv}},\theta_{a'}^{\xi\,\mathrm{adv}}), \tag{2.1}$$

coming from field theories such as long range[8] scalar or vector interaction. The $\mu_{aa'}$ are arbitrary constant numbers (that are equal to 1 in the purely retarded case, and to $\frac{1}{2}$ in the time-symmetric case). These formulas are used as boundary conditions for integrating (1.10d) by means of integrofunctional equations as follows:

$$\theta_a^\alpha=\sum_{a'}\mu_{aa'}\theta_a^\alpha(a';1)+(1-\mu_{aa'})\theta_a^\alpha(a';-1), \tag{2.2a}$$

$$\theta_a^\alpha(a';\epsilon)=R_{a'}[\lambda_{aa'}(\epsilon)]\theta^{*\alpha}_a(x_a^\beta-x_{a'}^\beta,\pi_a^\gamma,\pi_{a'}^\delta,\theta_{a'}^\xi)$$
$$+\int_0^{\lambda_{aa'}(\epsilon)}d\lambda\ R_{a'}(\lambda)\theta_a^\eta\frac{\partial}{\partial\pi^{a'\eta}}\theta_a^\alpha(a';\epsilon), \tag{2.2b}$$

where $R_{a'}$ acting on any function f is defined by

$$R_a(\lambda)f(x_b^\beta,\pi_c^\gamma)=f(x_b^\beta+\delta_b^a\lambda\,\pi_a^\beta,\pi_c^\gamma). \tag{2.3}$$

In the first term of (2.2b), $R_{a'}$ acts also on the arguments of $\theta_a^\xi;\epsilon$ is $+1$ (resp. -1) when in (2.1) a' is in retarded (resp. advanced) position with respect to a; the $\lambda_{aa'}(\epsilon)$ are solutions of the isotropic conditions

$$R_{a'}(\lambda)x_{aa'}^\alpha x_{aa'\alpha}=0, \tag{2.4}$$

where $x_{aa'}^\alpha\equiv x_a^\alpha-x_{a'}^\alpha$. Thus

$$\lambda_{aa'}(\epsilon)=(\pi_a^\alpha\pi_{a\alpha})^{-1}\{\pi^\alpha x_{aa'\alpha}+\epsilon$$
$$\times[(\pi_a^\alpha x_{aa'\alpha})^2-(x_{aa'}^\alpha x_{aa'\alpha})(\pi_a^\alpha\pi_{a\alpha})^{1/2}\}. \tag{2.5}$$

Equation (2.2b) can be solved by expanding accelerations in powers of appropriate parameters. For example, if $\theta^{*\alpha}_a(x_{aa'}^\beta,\pi_a^\gamma,\pi_{a'}^\delta,\theta_{a'}^\xi)$ contains the charge product $e_a e_{a'}$ in factor, and is expandable in power series of $\theta_{a'}^\xi$, we will postulate

$$\theta_a^\alpha = \sum_{n=1}^{\infty} \theta_{a\,n}^{\alpha}, \tag{2.6}$$

where $\theta_{a\,n}^{\alpha}$ has a product of $2n$ charges in factor. For $n \geqslant 2$ the computation of $\theta_{a\,n}^{\alpha}$ requires only the knowledge of $\theta_{a\,m}^{\alpha}$, $1 \leqslant m \leqslant n-1$:

$$\theta_{a\,n}^{\alpha} = \sum_{a'} \mu_{aa'} \theta_{a\,n}^{\alpha}(a';1) + (1-\mu_{aa'}) \theta_{a\,n}^{\alpha}(a';-1), \tag{2.7a}$$

$$\theta_{a\,n}^{\alpha}(a';\epsilon) = \Theta_{a\,n}^{\alpha} + \sum_{m=1}^{n-1} \int_0^{\lambda_{aa'}(\epsilon)} d\lambda R_{a'}(\lambda)\, \theta_{a'\,n-m}^{\beta} \times \frac{\partial}{\partial \pi^{a'\beta}} \theta_{a\,m}^{\alpha}(a';\epsilon), \tag{2.7b}$$

where $\Theta_{a\,n}^{\alpha}$ is the term of order n in the expansion of $R_{a'}[\lambda_{aa'}(\epsilon)]\theta^{*\alpha}_{a}(x^{\beta}_{aa'}, \pi^{\gamma}_{a}, \pi^{\delta}_{a'}, \theta^{\xi}_{a'})$. To first order, (2.7a) holds with simply

$$\theta_{a\,1}^{\alpha}(a';\epsilon) = R_{a'}[\lambda_{aa'}(\epsilon)]\theta^{*\alpha}_{a}(x^{\beta}_{aa'}, \pi^{\gamma}_{a}, \pi^{\delta}_{a'}, 0). \tag{2.8}$$

Interpretation of $\theta_{a\,1}^{\alpha}(a';\epsilon)$ is obvious: it is the retarded ($\epsilon = 1$) or advanced ($\epsilon = -1$) part of the acceleration of a due to a' as if, for each configuration $(x^{\beta}_{a'}, \pi^{\gamma}_{a'})$, a' were in uniform motion. It happens that, for scalar and vector interaction, $\theta_{a\,1}^{\alpha}(a';\epsilon)$ is independent of ϵ. The subsequent $\theta_{a\,n}^{\alpha}$, $n \geqslant 2$, bring successive corrections to this first approxiation.

In this method, the uniform motion thus constitutes the basic approximation for integrating the predicitivity conditions, and we obtain the accelerations explicitly in terms of the x's and π's. This form is appropriate for the Hamiltonian formulation of Sec. 3.

B. INTEGRATION IN SEMI-IMPLICIT FORM

In this method we look for accelerations as functions of positions, velocities, and accelerations themselves

$$\frac{du_a^\alpha}{d\tau_a} = W_a^\alpha(x_b^\beta, u_c^\gamma, A_d^\delta). \tag{2.9}$$

Of course, this does not mean that accelerations are part of the initial conditions. It does correspond to a second-order mechanics, only implying that one should invert

$$A_a^\alpha = W_a^\alpha(x_b^\beta, u_c^\gamma, A_d^\delta) \tag{2.10}$$

to obtain the accelerations in explicit form, namely as functions of positions and velocities.

Equations of type (2.9) could be suggested by the very presence of the accelerations as arguments in the Liénard–Wiechert type formulas

$$\frac{du_a^\alpha}{d\tau^a} = \sum_{a'} \mu_{aa'} A^{*\alpha}_{a}(x_a^\beta - x_{a'}^{\beta\,\mathrm{ret}}, u_a^\gamma, u_{a'}^{\delta\,\mathrm{ret}}, A_{a'}^{\xi\,\mathrm{ret}}) + (1-\mu_{aa'}) \times A^{*\alpha}_{a}(x_a^\beta - x_{a'}^{\beta\,\mathrm{adv}}, u_a^\gamma, u_{a'}^{\delta\,\mathrm{adv}}, A_{a'}^{\xi\,\mathrm{adv}}) \tag{2.11}$$

A possible theoretical advantage is that it might not always be possible to obtain explicit accelerations in closed form. A very peculiar example, that of the one-dimensional asymmetric electromagnetic interaction, shown exactly solvable by Hill and Rudd,[9] supports this conjecture: we do know the equations of the integral curves of the system under the form: $t_a = f_a\ (x_a$; first integrals); we thus have all we need to obtain the accelerations in explicit form by differentiating twice and eliminating the first integrals; however, the presence of transcendental functions in f_a prevents us from achieving this idea.

The true motivation is that we can expand the W_a^α in power series, and that these semi-implicit series contain more information, at equal number of terms, than the explicit series, as illustrated by two examples. The semi-implicit form comes to nothing more than regrouping differently the terms of the explicit series.

The predictivity conditions to be integrated will now read

$$\left(u^{a'\alpha}\frac{\partial}{\partial x_{a'}^{\alpha}} + A^{a'\alpha}\frac{\partial}{\partial x_{a'}^{\alpha}} + \dot{A}^{a'\alpha}\frac{\partial}{\partial A_{a'}^{\alpha}}\right) W_a^\beta = 0, \tag{2.12}$$

where $\dot{A}_{a'}^{\alpha}$ is $dA_{a'}^{\alpha}/d\tau_{a'}$, and is obtained by inversion of

$$\left(u^{a'\alpha}\frac{\partial}{\partial x_{a'}^{\alpha}} + A^{a'\alpha}\frac{\partial}{\partial u_{a'}^{\alpha}} + \dot{A}^{a'\alpha}\frac{\partial}{\partial A_{a'}^{\alpha}}\right) W_{a'}^\beta = \dot{A}_{a'}^{\beta}. \tag{2.13}$$

The corresponding basic approximation is now the relativistic uniformly accelerated motion

$$\frac{dA_{a'}^{\alpha}}{d\sigma} = A_{a'}^{2} u_{a'}^{\alpha} \quad (A_{a'}^{2} \equiv A_{a'}^{\beta} A_{a'\beta}). \tag{2.14}$$

Integration of this equation serves as a definition of the operator $S_{a'}$, replacing $R_{a'}$ of the preceding section. Let $(x_b^\beta, u_c^\gamma, A_d^\delta)$ be an "initial" configuration. Let particle a' evolve according to (2.14), and freeze all other particles. Let σ be the proper time measured along the trajectory of a', elapsed from the initial configuration. Then $S_{a'}$ is the identity on $x_a^\alpha, u_a^\beta, A_a^\gamma$, and

$$S_{a'}(\sigma)\, x_{a'}^{\alpha} = x_{a'}^{\alpha}(\sigma),\ S_{a'}(\sigma)\, u_{a'}^{\alpha} = u_{a'}^{\alpha}(\sigma),$$
$$S_{a'}(\sigma)\, A_{a'}^{\alpha} = A_{a'}^{\alpha}(\sigma). \tag{2.15}$$

$S_{a'}(\sigma) A_{a'}^{\alpha}$ is of course not to be confused with $S_{a'}(\sigma)\, W_{a'}^{\alpha}$. Note that

$$\partial_{a'} S_{a'}(\sigma) \equiv \frac{d}{d\sigma} S_{a'}(\sigma), \tag{2.16}$$

$$\partial_{a'} \equiv u^{a'\alpha}\frac{\partial}{\partial x_{a'}^{\alpha}} + A^{a'\alpha}\frac{\partial}{\partial u_{a'}^{\alpha}} + A_{a'}^{2} u^{a'\alpha}\frac{\partial}{\partial A_{a'}^{\alpha}}.$$

Let $\sigma_{aa'}(\epsilon)$ position the point of the trajectory of a' which is in retarded ($\epsilon = 1$) or advanced ($\epsilon = -1$) position with respect to a:

$$S_{a'}[\sigma_{aa'}(\epsilon)]x^{\alpha}_{aa'}x_{aa'\alpha}=0. \tag{2.17}$$

Important properties are

$$\partial_{a'}\sigma_{aa'}(\epsilon)=-1,$$
$$S_{a'}[\sigma_{aa'}(\epsilon)]\sigma_{aa'}(\epsilon)=0,$$
$$S_{a'}(\sigma_1)S_{a'}(\sigma_2)=S_{a'}[\sigma_1+S_{a'}(\sigma_1)\sigma_2]. \tag{2.18}$$

Write (2.12) as follows:

$$\partial_{a'}W^{\alpha}_{a}=-(\dot{A}^{\beta}_{a'}-A^{2}_{a}u^{\beta}_{a'})\frac{\partial}{\partial A^{a'\beta}}W^{\alpha}_{a}, \tag{2.19}$$

and, since computations must eventually end up by the inversion of $A^{\alpha}_{a}=W^{\alpha}_{a}$, integrate rather this equation

$$\partial_{a'}W^{\alpha}_{a}=-(\dot{A}^{\beta}_{a'}-W^{2}_{a'}u^{\beta}_{a'})\frac{\partial}{\partial A^{a'\beta}}W^{\alpha}_{a} \tag{2.20}$$

as follows:

$$W^{\alpha}_{a}=\sum_{a'}\mu_{aa'}W^{\alpha}_{a}(a';1)+(1-\mu_{aa'})W^{\alpha}_{a}(a';-1), \tag{2.21a}$$

$$W^{\alpha}_{a}(a';\epsilon)=S_{a'}[\sigma_{aa'}(\epsilon)]A^{*\alpha}_{a}(x^{\beta}_{aa'},u^{\gamma}_{a},u^{\delta}_{a'},A^{\xi}_{a'})$$
$$+\int_{0}^{\sigma_{aa'}(\epsilon)}d\sigma S_{a'}(\sigma)(\dot{A}^{\beta}_{a'}-W^{2}_{a}u^{\beta}_{a'})$$
$$\times\frac{\partial}{\partial A^{a'\beta}}W^{\alpha}_{a}(a';\epsilon). \tag{2.21b}$$

As in the explicit formalism, Eq. (2.21) can be solved step by step in powers of $g_{aa'}\equiv e_a e_{a'}$: that is why, on going from (2.19) to (2.20), we replaced $A^{2}_{a'}$ which, before inversion, does not contain the g's, by $W^{2}_{a'}$ which does. We thus postulate

$$W^{\alpha}_{a}=\sum_{N=1}^{\infty}\underset{N}{W}{}^{\alpha}_{a}. \tag{2.22}$$

A nice thing about the semi-implicit formalism is that $A^{*\alpha}_{a}$ contributes only to $\underset{1}{W}{}^{\alpha}_{a}$, though in the explicit formalism, $\theta^{*\alpha}_{a}$ contributed to all terms of the series since its argument $\theta^{\beta}_{a'}$ also had to be expanded in power series. For electromagnetism, we remark that $\underset{1}{W}{}^{\alpha}_{a}(a';1)=\underset{1}{W}{}^{\alpha}_{a}(a';-1)$.

Let us proceed to show that this method provides the same accelerations as the explicit formalism. First invert $\widetilde{A}^{\alpha}_{a}=W^{\alpha}_{a}(x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d})$ to get $\widetilde{A}^{\alpha}_{a}(x^{\beta}_{b},u^{\gamma}_{c})$, and define $\widetilde{A}^{\alpha}_{a}(a';\epsilon)(x^{\beta}_{b},u^{\gamma}_{c})$ as being equal to $W^{\alpha}_{a}(a';\epsilon)[x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d}(x^{\epsilon}_{c},u^{\xi}_{f})]$

We want to show that $\widetilde{A}^{\alpha}_{a}(a';\epsilon)=A^{\alpha}_{a}(a';\epsilon)$ [$A^{\alpha}_{a}(a';\epsilon)$ is obtained from $\theta^{\alpha}_{a}(a';\epsilon)$ of Eq. (2.2) according to the rule (1.19)]. Then evaluate (2.21) for $A^{\alpha}_{a}=\widetilde{A}^{\alpha}_{a}$, and set a' in retarded ($\epsilon=1$) or advanced ($\epsilon=-1$) position with respect to a which makes $\sigma_{aa'}(\epsilon)=0$ and yields

$$\widetilde{A}^{\alpha}_{a}(a';\epsilon)(x^{\beta}_{b},u^{\gamma}_{c})=A^{*\alpha}_{a}[x^{\beta}_{aa'},u^{\gamma}_{a},u^{\delta}_{a'},\widetilde{A}^{\epsilon}_{a'}(x^{\xi}_{d},u^{\eta}_{e})]$$
$$(\text{for } x^{0}_{aa'}=\epsilon(x^{i}_{aa'}x_{aai})^{1/2}). \tag{2.23}$$

Next set $A^{\beta}_{b}=\widetilde{A}^{\beta}_{b}$ in (2.13), and compare with the result of applying $u^{a'\beta}(\partial/\partial x^{\beta}_{a'})+\widetilde{A}^{a'\beta}(\partial/\partial u^{\beta}_{a'})$ on $\widetilde{A}^{\alpha}_{a'}=W^{\alpha}_{a'}(x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d})$ to get

$$\dot{A}^{\beta}_{a'}[x^{\alpha}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d}(x^{\epsilon}_{c},u^{\eta}_{f})]$$
$$=\left(u^{a'\xi}\frac{\partial}{\partial x^{\xi}_{a'}}+\widetilde{A}^{a'\xi}\frac{\partial}{\partial u^{\xi}_{a'}}\right)\widetilde{A}^{\beta}_{a'}(x^{\gamma}_{b},u^{\delta}_{c}). \tag{2.24}$$

Then evaluate

$$\left\{u^{a'\beta}\frac{\partial}{\partial x^{\beta}_{a'}}+A^{\alpha'\beta}\frac{\partial}{\partial u^{\beta}_{a'}}+[(A^{2}_{a'}-W^{2}_{a'})u^{a'\beta}+\dot{A}^{a'\beta}]\frac{\partial}{\partial A^{\beta}_{a'}}\right\}$$
$$\times W^{\alpha}_{a}(a';\epsilon)=0 \tag{2.25}$$

[of which (2.21b) is the integration] for $A^{\beta}_{b}=\widetilde{A}^{\beta}_{b}$. This yields with the help of (2.24)

$$\left\{u^{a'\beta}\frac{\partial}{\partial x^{\beta}_{a'}}+\widetilde{A}^{a'\beta}\frac{\partial}{\partial u^{\beta}_{a'}}+\left[\left(u^{a'\gamma}\frac{\partial}{\partial x^{\gamma}_{a'}}+\widetilde{A}^{a'\gamma}\frac{\partial}{\partial u^{\gamma}_{a'}}\right)\right]\widetilde{A}^{a'\beta}\right.$$
$$\left.\frac{\partial}{\partial\widetilde{A}^{\beta}_{a'}}\right\}\times W^{\alpha}_{a}(a';\epsilon)(x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d})=0 \tag{2.26}$$

or

$$\left(u^{a'\beta}\frac{\partial}{\partial x^{\beta}_{a'}}+\widetilde{A}^{a'\beta}\frac{\partial}{\partial u^{\beta}_{a'}}\right)\widetilde{A}^{\alpha}_{a}(a';\epsilon)(x^{\gamma}_{b},u^{\delta}_{c})=0. \tag{2.27}$$

Then postulate an expansion in powers of the coupling constant for $\widetilde{A}^{\alpha}_{a}(\widetilde{A}^{\alpha}_{a}=\Sigma_{n}\widetilde{A}^{\alpha}_{a})$ and proceed by recurrence by supposing that $\widetilde{A}^{\alpha}_{a}(a';\epsilon)=A^{\alpha}_{a}(a';\epsilon)$ has been proved up to order n (this is obviously true for $n=1$); thus, by linear combination, $\widetilde{A}^{\alpha}_{a}=A^{\alpha}_{a}$ is true up to the same order. Then the $(n+1)$st order term of (2.23) and (2.27) tells us that $\underset{n+1}{\widetilde{A}}{}^{\alpha}_{a}(a';\epsilon)$ and $\underset{n+1}{A}{}^{\alpha}_{a}(a';\epsilon)$ are equal since they satisfy the same equation with the same boundary condition. They are thus equal to all order

$$\widetilde{A}^{\alpha}_{a}(a';\epsilon)=W^{\alpha}_{a}(a';\epsilon)(x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d})=A^{\alpha}_{a}(a';\epsilon) \tag{2.28}$$

and, by linear combination

$$\widetilde{A}^{\alpha}_{a}=W^{\alpha}_{a}(x^{\beta}_{b},u^{\gamma}_{c},\widetilde{A}^{\delta}_{d})=A^{\alpha}_{a}. \tag{2.29}$$

First application: when two charges of opposite sign ($g=e_1e_2<0$) and equal masses m interacting according to Wheeler and Feynman electrodynamics describe the same circle, the radius of this circle is given in terms of the common velocity $v=\beta c$ by[10]:

$$r=-\frac{g}{4mv^{2}}P(\beta),\quad P(\beta)=1-\beta^{2}+5\beta^{4}\cdots. \tag{2.30}$$

Using $\underset{1}{A}{}^{\alpha}_{a}$ for the acceleration A^{α}_{a} allows to find correctly only the first term of $P(\beta)$ which thus could have been more simply obtained through nonrelativistic mechanics. The first relativistic correction [second term of $P(\beta)$] requires the computation of $\underset{1}{A}{}^{\alpha}_{a}+\underset{2}{A}{}^{\alpha}_{a}$ in the explicit formalism, though of only $\underset{1}{W}{}^{\alpha}_{a}$ in the semi-implicit formalism.

Second application: The one-dimensional and equal masses static case (acceleration for the special configuration $v_1=v_2=0$) shows that with terms only up to g^2 ($\underset{\text{I}}{W}{}^{\alpha}_{a}+\underset{\text{II}}{W}{}^{\alpha}_{a}$) we correctly obtain the acceleration up to order g^3 [4]:

$$a_1=a_2=gm^{-1}x^{-2}+g^2m^{-2}x^{-3}+\tfrac{3}{4}g^3m^{-3}x^{-4}. \tag{2.31}$$

3. SEVERAL QUESTIONS IN HAMILTONIAN FORMULATION

A. Review of Hamiltonian formulation of RPM in manifestly invariant formalism (Ref. 11)

To give a Hamiltonian formulation of a Poincaré invariant predictive system is to find a symplectic form Ω, namely a 2-form defined on the phase space of the system, regular ($\det\Omega\neq 0$), closed ($d\Omega=0$), and invariant by the $10+n$ vector fields $\Lambda=\mathbf{P}_\lambda, \mathbf{J}_{\lambda\mu}, \mathbf{H}_a$:

$$\mathscr{L}(\Lambda)\Omega=0, \tag{3.1}$$

where $\mathscr{L}(\ )$ is the Lie derivative. We know that to each such Λ leaving Ω invariant, we can associate a function $\Lambda=F(\Lambda)$ defined on the phase space, up to an additive constant, by

$$i(\Lambda)\Omega=-d\Lambda, \tag{3.2}$$

where $i(\ )$ denotes the inner product. We then can prove

$$\mathscr{L}(\Lambda_i)\Lambda_j=[\Lambda_i,\Lambda_j],$$
$$dF([\Lambda_i,\Lambda_j])=d[\Lambda_i,\Lambda_j], \tag{3.3}$$

where $[\Lambda_i,\Lambda_j]$ is the Poisson bracket of Λ_i and Λ_j according to Ω and $[\Lambda_i,\Lambda_j]$ the Lie bracket of Λ_i and Λ_j. Let P_λ, $\dot{J}_{\lambda\mu}$, H_a be the functions associated to $\mathbf{P}_\lambda$, $\mathbf{J}_{\lambda\mu}$, $\mathbf{H}_a$. (One can prove that all additive constants can be fixed). From (3.3), P_λ is a 4-vector, $\dot{J}_{\lambda\mu}$ a 4-tensor, and H_a scalars, and their Poisson brackets are homomorphic to their Lie brackets. Note in particular

$$[H_a,H_{a'}]=0. \tag{3.4}$$

For free particles, we have $\underset{0}{\Omega}=dx^{\alpha}_{a}\wedge d\pi^{a}_{\alpha}$ and we obtain for $\underset{0}{\Lambda}$:

$$\underset{0}{P}{}_{\lambda}=\sum_a \pi_{a\lambda},\quad \underset{0}{\dot{J}}{}_{\lambda\mu}=x_{a\lambda}\pi^{a}_{\mu}-x_{a\mu}\pi^{a}_{\lambda},$$
$$\underset{0}{H}{}_a=-\tfrac{1}{2}\pi^{\alpha}_{a}\pi_{a\alpha}. \tag{3.5}$$

Requiring:

$$\lim_{\lambda\to-\infty}\prod_a R_a(\lambda)\Omega=\underset{0}{\Omega}$$

entails:

$$\lim_{\lambda\to-\infty}\prod_a R_a(\lambda)\Lambda=\underset{0}{\Lambda}$$

which helps identifying P_λ and $\dot{J}_{\lambda\mu}$, respectively, with the energy-momentum 4-vector, and the generalized angular momentum 4-tensor of the system, when interaction is present. It can be proved that $H_a=-\frac{1}{2}\pi^{\alpha}_{a}\pi_{a\alpha}$, or, numerically speaking: $H_a=\frac{1}{2}m_a^2$.

The zero-interaction[12] theorem indicates that in a Hamiltonian formulation invariant by the complete symmetry group, particle positions x^{α}_{a} cannot be canonical variables, except for the case of free particles.[13]

A particular set of canonical coordinates up to first order in the charge product $g_{aa'}$ is provided by

$$\hat{p}^{\alpha}_{a}=\underset{0}{\pi}{}^{\alpha}_{a}+\underset{1}{p}{}^{\alpha}_{a},\quad \hat{q}^{\alpha}_{a}=\underset{0}{x}{}^{\alpha}_{a}+\underset{1}{\hat{q}}{}^{\alpha}_{a},$$
$$(\Omega=d\hat{q}^{\alpha}_{a}\wedge d\hat{p}^{a}_{\alpha}), \tag{3.6a}$$
$$\hat{p}^{\alpha}_{a}=\int_0^{-\infty}d\lambda R_a(\lambda)\underset{1}{\theta}{}^{\alpha}_{a},$$
$$\hat{q}^{\alpha}_{a}=-\int_0^{-\infty}d\lambda R_a(\lambda)\underset{1}{p}{}^{\alpha}_{a}, \tag{3.6b}$$

giving

$$P_\lambda=\sum_a \hat{p}_{a\lambda},\quad \dot{J}_{\lambda\mu}=\hat{q}_{a\lambda}\hat{p}^{a}_{\mu}-\hat{q}_{a\mu}\hat{p}^{a}_{\lambda}. \tag{3.6c}$$

One can make a canonical transformation from this set to another set: $(\hat{q}^{\alpha}_{a},\hat{p}^{\alpha}_{a})\to(q^{\alpha}_{a},p^{\alpha}_{a})$; then

$$P_\lambda=\sum_a p_{a\lambda},\quad \dot{J}_{\lambda\mu}=q_{a\lambda}p^{a}_{\mu}-q_{a\mu}p^{a}_{\lambda}, \tag{3.7}$$

and H_a is $-\frac{1}{2}\pi^{\alpha}_{a}\pi_{a\alpha}$, where π^{α}_{a} is reexpressed in terms of q^{β}_{b} and p^{γ}_{c}.

B. Poisson bracket of position variables of each particle

From the zero-interaction theorem we cannot have altogether when interaction is present

$$[x^{\alpha}_{a},x^{\beta}_{b}]=0. \tag{3.8}$$

However we can ask if we can have the less restrictive conditions

$$[x^{\alpha}_{a},x^{\beta}_{a}]=0. \tag{3.9}$$

up to first order in $g_{aa'}$. Inverting (3.6a) up to that order, (3.9) means

$$\left[\hat{q}^{\alpha}_{a}-\underset{1}{\hat{q}}{}^{\alpha}_{a},\hat{q}^{\beta}_{a}-\underset{1}{\hat{q}}{}^{\beta}_{a}\right]=0 \tag{3.10}$$

or

$$\frac{\partial}{\partial\pi^{a\beta}}\underset{1}{\hat{q}}{}_{a\alpha}-\frac{\partial}{\partial\pi^{a\alpha}}\underset{1}{\hat{q}}{}_{a\beta}=0 \tag{3.11}$$

which guarantees that functions $\underset{1}{\Sigma}{}_{a}(x^{\beta}_{b},\pi^{\gamma}_{c})$ exist such that

$$\underset{1}{\Sigma}{}_{a}=\int\underset{1}{q}{}^{\alpha}_{a}d\pi_{a\alpha}. \tag{3.12}$$

Let us introduce $\underset{1}{L}{}_{a}$ by (with $D_a\equiv\pi^{\alpha}_{a}\partial/\partial x^{a\alpha}$)

$$\underset{1}{L}{}_{a}=D_a\underset{1}{\Sigma}{}_{a}$$

$$= -\pi_a^\alpha \frac{\partial}{\partial x^{a\alpha}}$$

$$\int d\pi_{a\beta} \int_0^{-\infty} d\lambda R_a(\lambda) \int_0^{-\infty} d\lambda' R_a(\lambda') \theta_{1\,a}^{\beta}. \tag{3.13}$$

It is then easy to see that

$$\theta_{1\,a}^{\alpha} = \left[\frac{\partial}{\partial x_\alpha^a} - \left(\pi_a^\beta \frac{\partial}{\partial x^{a\beta}}\right)\frac{\partial}{\partial \pi_\alpha^a}\right] L_{1\,a} \tag{3.14}$$

but these equations are precisely the Euler equations at the order considered of the following private variational principles:

$$\delta_a \int L_a \, d\lambda_a = 0, \quad L_a = \tfrac{1}{2}\pi_a^\alpha \pi_{a\alpha} + L_{1\,a}, \tag{3.15}$$

where δ_a means that only x_a^α (and π_a^α) are varied, $x_{a'}^\alpha, \pi_{a'}^\alpha$, being kept fixed.

In other words, the nullity of Poisson brackets of position variables of each particle up to first order implies the existence of private Lagrangians up to first order admitting particle position x_a^α as private Lagrangian variables.

Conversely, n such private Lagrangians L_a being given—satisfying $(\pi_a^\alpha \partial/\partial \pi^{a\alpha}) L_{1\,a} = L_{1\,a}$ and $D_{a'} L_{1\,a} = 0$ to guarantee, respectively, $\pi_a^\alpha \theta_{a\alpha} = 0$ and $D_{a'} \theta_{1\,a}^{\alpha} = 0$—one can carry out n private canonical transformations from x_a^α, $p_{a\alpha} = \partial L_a / \partial \pi^{a\alpha}$ to new variables $\hat{q}_a^\alpha$, $\hat{p}_\alpha^a$ which will be, up to first order, canonical variables for the common symplectic form $\Omega = d\hat{q}_a^\alpha \wedge d\hat{p}_\alpha^a$ since they are built to satisfy $\pounds(\mathbf{H}_b)\hat{q}_a^\alpha = \delta_{ab}\hat{p}_b^\alpha$, $\pounds(\mathbf{H}_b)\hat{p}_a^\alpha = 0$, implying $\pounds(\mathbf{H}_b)\Omega = 0$:

$$x_a^\alpha \to \hat{q}_a^\alpha = x_a^\alpha + \frac{\partial}{\partial \pi_\alpha^a} \Sigma_{1\,a},$$

$$p_{a\alpha} \to \hat{p}_{a\alpha} = p_{a\alpha} - \frac{\partial}{\partial x^{a\alpha}} \Sigma_{1\,a},$$

where $\Sigma_{1\,a}$ is defined by

$$\Sigma_{1\,a} = -\int_0^{-\infty} d\lambda \, R_a(\lambda) L_{1\,a}. \tag{3.16}$$

We thus have not only $[x_a^\alpha, x_a^\beta] = 0$ but also $[x_a^\alpha, p_a^\beta] = \delta^{\alpha\beta}$ and $[p_a^\alpha, p_a^\beta] = 0$, these Poisson brackets being computed up to first order according to the common symplectic form.

The interest of this question is that one meets the above properties for scalar and vector interaction, of short or long range, because we do have in the corresponding field theories one variational principle per particle, admitting particle position as private Lagrangian variables, and providing Lagrangians L_a through the uniform motion approximation for particles not varied. Let us illustrate this on electromagnetism, for which field theory gives

$$\delta_a \int \left[\tfrac{1}{2}\pi_a^\alpha \pi_{a\alpha} + e_a \pi_a^\alpha \sum_{a'} \left(\mu_{aa'} \frac{e_{a'} \pi_{a'\alpha}^{\text{ret}}}{|(x_a^\beta - x_{a'}^{\beta\,\text{ret}})\, \pi_{a'\beta}^{\text{ret}}|} + (1 - \mu_{aa'}) \frac{e_{a'} \pi_{a'\alpha}^{\text{adv}}}{|(x_a^\beta - x_{a'}^{\beta\,\text{adv}})\, \pi_{a'\beta}^{\text{adv}}|} \right) \right] d\lambda_a = 0 \tag{3.17}$$

and for which we get

$$L_a = \tfrac{1}{2}\pi_a^\alpha \pi_{a\alpha} + \sum_{a'} \frac{e_a e_{a'} \pi_a^\alpha \pi_{a'\alpha}}{[-x_{aa'}^2 \pi_{a'}^2 + (x_{aa'}^\beta \pi_{a'\beta})^2]^{1/2}}. \tag{3.18}$$

C. Lagrangians, canonical transformations, and Hamilton–Jacobi equations

These three simple notions are reconsidered in the frame of the Hamiltonian formulation of PRM where we have one Hamiltonian per particle. We start by introducing one Lagrangian per particle, but these are not to be confused with the ones of the preceding subsection.

The canonical equations of motion, coming from the invariance of Ω by the $\mathbf{H}_a$

$$\frac{dq_b^\beta}{d\lambda_a} = \frac{\partial H_a}{\partial p_\beta^b}, \qquad \frac{dp_\beta^b}{d\lambda_a} = -\frac{\partial H_a}{\partial q_b^\beta} \tag{3.19a}$$

are compatible in virtue of $[H_a, H_{a'}] = 0$, and their solution gives q_a^α and p_b^β as functions of the initial conditions $q_{0\,c}^\gamma$ and $p_{0\,d}^\delta$ and of the n parameters λ_a; the solution is thus a n-hypersurface tangent to the n field vectors $\mathbf{H}_a$.

For each value of the index a invert (3.19a) to get p_b^β in terms of q_c^γ and $dq_d^\delta/d\lambda_a$. The expressions $p_b^{(a)\beta}(q_c^\gamma, dq_d^\delta/d\lambda_a)$ obtained for different a, are not the same, but they of course become equal functions of the λ's when the q_c^γ are replaced by their expressions in terms of the initial conditions and the λ's.

$$p_b^{(a)\beta}\left[q_c^\gamma(\lambda_a), \frac{dq_e^\delta(\lambda_f)}{d\lambda_a}\right] = p_b^{(a')\beta}\left[q_c^\gamma(\lambda_d), \frac{dq_e^\delta(\lambda_f)}{d\lambda_{a'}}\right]. \tag{3.20}$$

Then construct the Lagrangians L_a, Legendre transformed of each Hamiltonian

$$L_a\left(q_b^\beta, \frac{dq_c^\gamma}{d\lambda_a}\right) = p_\beta^{(a)b} \frac{dq_b^\beta}{d\lambda_a} - H_a(q_b^\beta, p_\gamma^{(a)c}). \tag{3.21}$$

The L_a satisfy

$$\frac{\partial L_a}{\partial q_b^\beta} = -\frac{\partial H_a}{\partial q_b^\beta}, \qquad \frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)} = p_\beta^{(a)b} \tag{3.22a,b}$$

and (3.19b) implies

$$\frac{d}{d\lambda_a}\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)}=\frac{\partial L_a}{\partial q_b^\beta}. \tag{3.23}$$

The proposed extremum action principle has the form $\delta A=0$ with

$$A=\int_{(\lambda_{i,f})} L_a d\lambda^a. \tag{3.24}$$

A depends on the functions $q_a^\alpha(\lambda_b)$ chosen to evaluate it, but, presenting itself as a curvilinear integral in the space $(\lambda_1,\lambda_2,\ldots,\lambda_n)$, it depends also *a priori* on the chosen integration path $\lambda_a(\lambda)$ parametrized by one parameter λ varying from an initial value λ_i to a final value λ_f; we set $\lambda_{ai}\equiv\lambda_a(\lambda_i),\lambda_{af}\equiv\lambda_a(\lambda_f)$. The action variation δA due to variations $\delta q_a^\alpha(\lambda_b)$ and $\delta\lambda_a(\lambda)$ is

$$\delta A=\sum_a\int d\lambda_a\frac{d}{d\lambda_a}\left[\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)}\delta q_b^\beta\right]+L_a\delta\lambda^a\Big|_i^f$$

$$+\sum_a\int d\lambda_a\,\delta q_b^\beta\left[\frac{\partial L_a}{\partial q_b^\beta}-\frac{d}{d\lambda_a}\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)}\right]$$

$$+\sum_{a,a'}\int\delta\lambda_a\,d\lambda_{a'}\left(\frac{dL_{a'}}{d\lambda_a}-\frac{dL_a}{d\lambda_{a'}}\right). \tag{3.25}$$

Now suppose that the variation $\delta q_a^\alpha(\lambda_b)$ occurs about a solution $q_a^\alpha(\lambda_b)$ of (3.23), and that both types of variation vanish at the end points

$$(\delta q_a^\alpha)(\lambda_{bi})=(\delta q_a^\alpha)(\lambda_{cf})=0, \tag{3.26a}$$

$$(\delta\lambda_a)(\lambda_i)=(\delta\lambda_a)(\lambda_f)=0, \tag{3.26b}$$

then, in virtue of (3.22b) and (3.20), $p_\beta^{(a)b}=p_\beta^{(a')b}=p_\beta^b$ and the first term of δA integrates to $p_\beta^b\delta q_b^\beta\big|_i^f$ and vanishes by virtue of (3.26a). The second term vanishes by virtue of (3.26b), and the third one is zero by (3.23). At last $[H_a,H_{a'}]=0$ gives, using (3.22a), (3.19a), (3.20), and (3.22b)

$$0=\frac{\partial H_a}{\partial q_b^\beta}\frac{\partial H_{a'}}{\partial p_\beta^b}-\frac{\partial H_{a'}}{\partial q_b^\beta}\frac{\partial H_a}{\partial p_\beta^b}$$

$$=-\frac{\partial L_a}{\partial q_b^\beta}\frac{dq_b^\beta}{d\lambda_{a'}}+\frac{\partial L_{a'}}{\partial q_b^\beta}\frac{dq_b^\beta}{d\lambda_a}$$

$$=-\left(\frac{\partial L_a}{\partial q_b^\beta}\frac{dq_b^\beta}{d\lambda_{a'}}+\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_{a'}}\right)}\frac{d^2q_b^\beta}{d\lambda_{a'}d\lambda_a}\right)$$

$$+\left(\frac{\partial L_{a'}}{\partial q_b^\beta}\frac{dq_b^\beta}{d\lambda_a}+\frac{\partial L_{a'}}{\partial\left(\frac{dq_b^\beta}{d\lambda_{a'}}\right)}\frac{d^2q_b^\beta}{d\lambda_{a'}d\lambda_a}\right)$$

$$=-\frac{dL_a}{d\lambda_{a'}}+\frac{dL_{a'}}{d\lambda_a}. \tag{3.27}$$

In other words, δA is zero for a variation δq_a^α—vanishing at the end points—of the solution q_a^α and for the variation of any integration path $\lambda_a(\lambda)$ with the same end points since, finally, from (3.27) which is an integrability relation, A is path independent.

The converse goes as follows: Some $L_a(q_b^\beta,dq_c^\gamma/d\lambda_a)$ being given, require that they define the same moments

$$\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)}=\frac{\partial L_{a'}}{\partial\left(\frac{dq_b^\beta}{d\lambda_{a'}}\right)}. \tag{3.28}$$

This constitutes a set of $4n(n-1)$ relations among the $4n+4n^2$ variables of the $(q_a^\alpha,dq_b^\beta/d\lambda_c)$ space. Thus the entire motion must lay on a $(4n+4n^2)-4n(n-1)=8n$-dimensional hypersurface. Then write $\delta A=0$ with (3.26). The first two terms of (3.25) vanishes as before. The fourth term

$$\frac{dq_b^\beta}{d\lambda_a}\frac{\partial L_{a'}}{\partial q_b^\beta}-\frac{dq_b^\beta}{d\lambda_{a'}}\frac{\partial L_a}{\partial q_b^\beta}+\frac{d^2q_b^\beta}{d\lambda_a\,d\lambda_{a'}}$$

$$\times\left(\frac{\partial L_{a'}}{\partial\left(\frac{dq_b^\beta}{d\lambda_{a'}}\right)}-\frac{\partial L_a}{\partial\left(\frac{dq_b^\beta}{d\lambda_a}\right)}\right)=0. \tag{3.29}$$

must be restricted by $p_\beta^{(a')b}=p_\beta^{(a)b}$, thus implying that the Hamiltonians H_a, Legendre transformed of the L_a, should have vanishing Poisson brackets. Finally Euler equations follow from the third term: it is easy to see that they respect the constraints (3.28), and entail Eq. (3.19).

Now two points $(q_{ai}^\alpha,\lambda_{bi})$ and $(q_{af}^\alpha,\lambda_{bf})$ being given in the $5n$-dimensional evolution space (q_a^α,λ_b), there is in general only one n-hypersurface $q_a^\alpha=f_a^\alpha(\lambda_b)$ satisfying (3.23) and passing through these two points. Let us use it to evaluate the action which we know to be independent of the integration path $\lambda_a(\lambda)$. The variation undergone by $A(q_{ai}^\alpha,q_{af}^\alpha,\lambda_{bi},\lambda_{bf})$ when both end points are varied is

$$\delta A=p_b^\beta\delta q_b^\beta+L_a\delta\lambda^a\Big|_i^f \tag{3.30}$$

whence, with obvious notations

$$\frac{\partial A}{\partial q_{af}^\alpha}=p_{af}^a,\quad\frac{\partial A}{\partial\lambda_{af}}=-H_a(q_{bf}^\beta,p_{\gamma f}^c) \tag{3.31}$$

$$\frac{\partial A}{\partial q_{ai}^\alpha}=-p_{ai}^a,\quad\frac{\partial A}{\partial\lambda_{ai}}=H_a(q_{bi}^\beta,p_{\gamma i}^c). \tag{3.31}$$

We thus have constructed a common solution to the n equations $H_a(q_b^\beta,\partial A/\partial q_c^\gamma)+\partial A/\partial\lambda_a=0$; it actually is a complete integral depending on $4n$ parameters q_{ai}^α. The n parameters λ_{ai} are irrelevant since, owing to the H_a being first integrals, A depends on λ_{af} and λ_{bi} only through the differences $\lambda_{af}-\lambda_{ai}$.

Now one can carry out a canonical transformation in phase space as usual: S being a function of q_a^α, P_b^β, λ_c, define new canonical variables through

$$p^{\alpha}_{a}=\frac{\partial S}{\partial q^{\alpha}_{a}},\quad Q^{\alpha}_{a}=\frac{\partial S}{\partial P^{a}_{\alpha}}. \tag{3.32}$$

The new Hamiltonian are then

$$K_a(Q^{\beta}_{b},\ P^{c}_{\gamma},\ \lambda_d)=H_a+\frac{\partial S}{\partial \lambda_a} \tag{3.33}$$

and are shown to satisfy

$$[K_a,\ K_{a'}]+\frac{\partial K_a}{\partial \lambda_{a'}}-\frac{\partial K_{a'}}{\partial \lambda_a}=0. \tag{3.34}$$

Hamilton–Jacobi equations are obtained as usual by asking that the new Hamiltonians K_a be zero, a choice trivially satisfying (3.34)

$$H_a\left(q^{\beta}_{b},\ \frac{\partial S}{\partial q^{\gamma}_{c}}\right)+\frac{\partial S}{\partial \lambda_a}=0. \tag{3.35}$$

This set of HJ equations constitutes a system of n first-order compatible partial differential equations on one function S of the $5n$ variables q^{α}_{a}, λ_b. Thus a complete integral depends on $5n-(n-1)=4n+1$ arbitrary constants, one of which is purely additive since S itself does not appear in the system

$$S=S(q^{\alpha}_{a},\ \lambda_b, a_i)+a,\quad i=1,2,\ldots,4n. \tag{3.36}$$

Writing $\partial S/\partial q^{\alpha}_{a}=p^{a}_{\alpha}$, $\partial S/\partial a_i=b^{i}$ defines

$$q^{\alpha}_{a}=f^{\alpha}_{a}(\lambda_b,a_i,\ b^{j}),\quad p^{\alpha}_{a}=g^{\alpha}_{a}(\lambda_b,a_i,b^{j}) \tag{3.37}$$

and these functions are easily shown to satisfy the systems of characteristics of the system of HJ equations, namely the canonical equations (3.19). Naturally, inversion of (3.37) yields functions a_i and b^j of q^{α}_{a}, f^{β}_{b}, λ_c satisfying:

$$[a_i,a_j]=0,\ [b^{i},b^{j}]=0,\ [b^{i},a_j]=\delta^{i}_{j}, \tag{3.38}$$

$$[a_i,H_a]+\frac{\partial a_i}{\partial \lambda_a}=0,\ [b^{i},H_a]+\frac{\partial b^{i}}{\partial \lambda_a}=0,$$

so that, as expected, S is the generating function of a canonical transformation from q^{α}_{a}, p^{β}_{b} towards a_i, b^j that are first integrals. Furthermore

$$\frac{dS}{d\lambda_a}=\frac{dq^{\beta}_{b}}{d\lambda_a}\frac{\partial S}{\partial q^{\beta}_{b}}+\frac{\partial S}{\partial \lambda_a}$$

$$=p^{b}_{\beta}\frac{dq^{\beta}_{b}}{d\lambda_a}-H_a=L_a. \tag{3.39}$$

Thus

$$S=\int L_a\,d\lambda^{a}+\text{constant}, \tag{3.40}$$

where f^{β}_{b} is $p^{\beta}_{b}(\lambda_c,a_i,b^{j})$ and where, after integration, the b^j are expressed in terms of q^{α}_{a}, λ_b, a_i.

Since the H_a are numerically equal to $\frac{1}{2}m^{2}_{a}$, a separation of variables is always possible under the form

$$S(q^{\alpha}_{a},\lambda_b)=W(q^{\alpha}_{a})-\sum_{a}\tfrac{1}{2}m^{2}_{a}\lambda_a, \tag{3.41}$$

where W is solution of

$$H_a\left(q^{\beta}_{b},\ \frac{\partial W}{\partial q^{\gamma}_{c}}\right)=\tfrac{1}{2}m^{2}_{a}. \tag{3.42}$$

If we consider these equations as an approximation of geometrical optics of a quantum mechanics to be built, we see that we should expect n evolution equations on the same n-point dependent wavefunction

$$\hat{H}_a\Psi=\tfrac{1}{2}m^{2}_{a}\Psi. \tag{3.43}$$

To first order in the coupling constant, such a mechanics has been built independently by Bel.[14]

D. Canonical formulation of the separation of external and internal motions

This separation is made in the manifestly predictive formalism. Let us indicate first how to go from the Hamiltonian formulation in the manifestly invariant formalism to the one in the manifestly predictive formalism.[11]

Let a bar denote the restriction on the hypersurface of equation

$$x^{0}_{a}=0,\ \pi^{i}_{a}=m_a v^{i}_{a}(1-v^{2}_{a})^{-1/2},\ \pi^{0}_{a}=m_a(1-v^{2}_{a})^{-1/2}, \tag{3.44}$$

where the m_a are fixed. The restriction of $\Omega=dq^{\alpha}_{a}\wedge dp^{a}_{\alpha}$ is $\Sigma=\bar{\Omega}=d\bar{q}^{\alpha}_{a}\wedge d\bar{p}^{a}_{\alpha}$. Σ can be shown to be invariant by the 10 vector fields $\mathbf{H}$, $\mathbf{P}_i$, $\mathbf{J}_j$, $\mathbf{K}_k$ given in (1.7), the associated functions through Σ being, respectively, given in terms of the functions P_λ, $J_{\lambda\mu}$ associated to $\mathbf{P}_\lambda$, $\mathbf{J}_{\lambda\mu}$ through Ω by

$$H=-\bar{P}_0,\ P_i=\bar{P}_i,\ \dot{J}_i=\tfrac{1}{2}\delta^{jk}_{i}J_{jk},\ K_i=-J_{i0}. \tag{3.45}$$

The $2n$ constraints $x^{0}_{a}=0$, $\pi^{\alpha}_{a}\pi_{a\alpha}=-m^{2}_{a}$ show that there exist $8n-2n=6n$ independent functions q^{i}_{a} and p^{j}_{b} of x^{k}_{c}, v^{l}_{d} and m_e such that $\Sigma=dq^{i}_{a}\wedge dp^{a}_{i}$.

The separation of external and internal motions consists first in choosing some new canonical variables, called external variables, whose motion is trivial and which generalize at the relativistic level some characteristic properties of the Newtonian center of mass. It is well known that P_i, the total linear momentum and

$$Q^{i}=\frac{K^{i}+P^{i}t}{H}-\frac{\epsilon^{i}_{jk}P^{j}(\epsilon^{k}_{lm}P^{l}K^{m}+\dot{J}^{k}H)}{Hh(H+h)},$$

$$h\equiv(H^{2}-P^{i}P_{i})^{1/2}, \tag{3.46}$$

the center of spin,[15] form such a pair:

$$[Q^{i},Q^{j}]=0,\ [Q^{i},P_j]=\delta^{i}_{j},\ [P_i,\ P_j]=0, \tag{3.47}$$
$$[Q^{i},\dot{J}_j]=\epsilon^{i}_{jk}Q^{k},\ [P_i,\dot{J}_j]=\epsilon_{ij}{}^{k}P_k,$$
$$[Q^{i},H]=H^{-1}P^{i},\ [P_i,H]=0.$$

Then define the internal symplectic form by

$$\sigma=\Sigma-dQ^{i}\wedge dP_i. \tag{3.48}$$

Σ is of rank $6n$; computation shows that there are six independent vector fields $\mathbf{P}_i$ and $\mathbf{k}_j$ whose interior product with σ vanishes

$$\mathbf{k}_j = \mathbf{K}_j - Q_j \mathbf{H} - (H+h)^{-1} \epsilon_j{}^{kl} P_k \dot{\mathbf{J}}_l, \qquad (3.49)$$
$$i(\mathbf{P}_i)\sigma = 0, \quad i(\mathbf{k}_j)\sigma = 0.$$

Thus σ is of rank $6(n-1)$; and it is closed ($d\sigma = 0$). From Darboux' theorem there exist $6(n-1)$ independent functions q'^i_a and p'^i_a, called the internal variables, such that σ can be written as

$$\sigma = dq'^i_a \wedge dp'^a_i, \quad a = 2,3,\ldots,n. \qquad (3.50)$$

From (3.49) and (3.50), the internal variables are thus solutions of

$$\mathscr{L}(\mathbf{P}_j) q'^i_a = 0, \quad \mathscr{L}(\mathbf{P}_j) p'^i_a = 0 \qquad (3.51a)$$
$$\mathscr{L}(\mathbf{k}_j) q'^i_a = 0, \quad \mathscr{L}(\mathbf{k}_j) p'^i_a = 0, \qquad (3.51b)$$

to which we add the condition that they should behave as vector components under the rotation group (which is compatible with the preceding relations)

$$\mathscr{L}(\dot{J}_j) q'^i_a = -\epsilon^i_{jk} q'^k_a, \quad \mathscr{L}(\dot{J}_j) p'^i_a = -\epsilon^i_{jk} p'^k_a. \qquad (3.51c)$$

This allows

$$\dot{J}_i = \epsilon_{ij}{}^k (Q^j P_k + q'^j_a p'^a_k). \qquad (3.52)$$

The general solution of (3.51a,c) is easy to write. To find the boundary conditons to integrate (3.51b) we start from $\Sigma = dq^i_a \wedge dp^a_i$. Let a bar now denote the restriction to the hypersurface $P_i = 0$. To do this, particularize arbitrarily one particle, say particle 1, by writing $p^i_1 = -\sum_{a=2}^{n} p^i_a$; we obtain

$$\bar{\Sigma} = d(\bar{q}^i_a - \bar{q}^i_1) \wedge d\bar{p}^a_i. \qquad (3.53)$$

On the other hand, the restriction of $\Sigma = dQ^i \wedge dP_i + dq'^i_a \wedge dp'^a_i$, $a = 2,3,\ldots n$, gives

$$\bar{\Sigma} = d\bar{q}'^i_a \wedge d\bar{p}'^a_i. \qquad (3.54)$$

The boundary conditions are thus, comparing (3.53) and (3.54):

$$q'^i_a = q^i_a - q^i_1, \quad p'^a_i = p^a_i \text{ when } P_j = 0 \qquad (3.55)$$

One can integrate (3.51b) by means of integrofunctional equations respecting the above boundary conditions.

One shows at last that the internal Hamiltonian defined as $h = (H^2 - P^i P_i)^{1/2}$ is independent of Q^i and P_j, and is a rotation-invariant function of the internal variables. Thus

$$H(Q^i, P_j, q'^k_a, p'_{ab}) = [P^i P_i + h^2(q'^i_a q'_{bi} q'^j_d p'_{dj} p'^k_e p'_{pk})]^{1/2}. \qquad (3.56)$$

4. CONCLUSION

The equations of PRM have been integrated in a semi-implicit form by means of coupled integrofunctional equations which respect the boundary conditions offered by field theories. They allow to compute the accelerations step by step, by postulating an expansion in powers of a parameter, a coupling constant for example. Inversion yields the accelerations of the explicit formalism; but two examples show that one obtain better results, at equal number of terms, than in the explicit formalism.

In the Hamiltonian formulation of PRM, in which the complete symmetry group is canonically represented, particle positions cannot in general be canonical variables. However $[x^\alpha_a, x^\beta_a]$ vanishes at the two lowest orders in the coupling constant as a consequence of the existence in field theories of private variational principles each admitting the position variables of a particle as private Lagrangian variables.

For a solution of the problem, the action, which presents itself as a curvilinear integral, does not depend on the integration path, and is stationary with respect to a variation of the solution.

The theory of Hamilton–Jacobi leads to as many compatible partial differential equations on the same generating function as particles existing in the system.

The interest of the separation of external and internal motions is to isolate six canonical external variables whose motion is simple since the system as a whole behaves as a free particle, thus leaving $6(n-1)$ nontrivial internal canonical degrees of freedom.

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[1] $a, b, c\cdots$ are the label of the particles and run from 1 to n unless otherwise stated; a' is always different from a, b' from $b,\ldots;i,j,k\cdots$ are spatial indices running from 1 to 3; $\alpha,\beta,\gamma\cdots\lambda,\mu$ are spatio-temporal indices and run from 0 to 3. The first two sorts of indices are raised and lowered without change in sign. Signature of space–time M_4 is $+2$, and its metric tensor is designated by $\eta_{\lambda\mu}$ Einstein convention is used for the three sorts of indices when in alternate position.

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Canonical Fourier transforms

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An analog of the Fourier–Plancherel transformation is developed which maps to themselves the "square-traceable" operators in the von Neumann algebra generated by a quantum-mechanical canonical pair (p,q). The role of translation-invariant integral is played by the trace. The Fourier transform is given formally by

$$\hat{X}(p',q') = \sin\alpha \,\mathrm{tr}_{p,q}\, e^{\,i\alpha(pp'+qq')} X(p,q),$$

where α is a fixed parameter in the interval of $(0,\pi)$. Comparisons are made with other Fourier-type transformations associated with a canonical pair.

1. INTRODUCTION

Let p and q be a canonical pair of quantum-mechanical momentum and position operators, that is, self-adjoint operators satisfying the Weyl relation

$$e^{isp}e^{itq} = e^{ist}e^{itq}e^{isp} \quad (s,t\in\mathbb{R}). \tag{1.1}$$

By the von Neumann uniqueness theorem, the von Neumann algebra $N(p,q)$ generated by p and q (that is, the von Neumann algebra generated by the unitary operators $\{e^{isp}: s\in\mathbb{R}\}$ and $\{e^{itq}: t\in\mathbb{R}\}$) is isomorphic to the algebra $B(L^2(\mathbb{R}))$ of all bounded operators on the Hilbert space $L^2(\mathbb{R})$, under a *canonical isomorphism* ν mapping each e^{isp} to e^{isp_0} and each e^{itq} to e^{itq_0}, *where* p_0 and q_0 are the *Schrödinger canonical pair*, that is, $p_0 = -id/dt$ and q_0 is multiplication by the coordinate variable t. In particular $N(p,q)$ is thus a type I factor and possesses a faithful normal semi-finite trace τ which is unique to within rescaling.

For arbitrary a and $b\in\mathbb{R}$, the operators $p+a$ and $q+b$ form a second canonical pair which generate the same von Neumann algebra $N(p,q)$, and hence there is an automorphism $T_{a,b}$ of $N(p,q)$ mapping each e^{isp} to $e^{is(p+a)}$ and each e^{itq} to $e^{it(q+b)}$. We call $T_{a,b}$ *translation through* (a,b). Since every automorphism of the type I factor $N(p,q)$ is inner, for arbitrary $X\in N(p,q)$ we have

$$\tau(T_{a,b}X) = \tau X,$$

that is, the trace τ is *translation-invariant*.

Our purpose in this work is to develop an analog of the Fourier–Plancherel transformation on $L^2(\mathbb{R})$ which acts in the Hilbert space $L^2(p,q)$ of "square-traceable" operators in $N(p,q)$ [that is, pre-images under the canonical isomorphism of Hilbert-Schmidt operators on $B(L^2(\mathbb{R}))$], in which the trace τ plays the role of the translation-invariant Lebesgue measure on $\mathbb{R}$. For suitably restricted $X\in L^2(p,q)$ the transform of X is given by

$$\hat{X} = \sin\alpha\,\tau_1 \exp[-i\alpha(p\otimes p + q\otimes q)]X\otimes 1.$$

Here α is a fixed parameter in the open interval $(0,\pi)$, and τ_1 denotes the "partial trace" from $N(p,q)\otimes N(p,q)$ to $N(p,q)$ (this is defined in Sec. 2). Abusing notation, we may write this in the form

$$\hat{X}(p',q') = \sin\alpha\ \mathrm{tr}_{p,q}\exp[-i\alpha(pp'+qq')]X(p,q),$$

where p' and q' form a (mutually commuting) copy of the canonical pair p and q, and the functional notation indicates membership of the corresponding von Neumann algebra. It will be shown that the transformation so defined extends uniquely to an isometry F_α from $L^2(p,q)$ onto itself, and that its inverse is given, for suitably restricted $\hat{X}\in L^2(p,q)$, by

$$X(p,q) = \sin\alpha\,\mathrm{tr}_{p'q'}\exp[i\alpha(pp'+qq')]\hat{X}(p',q').$$

In a series of works[1-3] it has been shown, in effect, that the map from suitably restricted operators in $N(p,q)$ to functions on $\mathbb{R}^2$,

$$X\to\Xi \quad \Xi(s,t) = (\gamma/2\pi)\tau\exp[-i\gamma(sp+tq)]X$$

(here γ is a fixed real nonzero parameter), extends to a unique isometry U_γ, the *Fourier–Plancherel–Weyl* transformation, from $L^2(p,q)$ onto $L^2(\mathbb{R}^2)$, whose inverse acts on suitable functions on $\mathbb{R}^2$ as

$$\Xi\to X = (\gamma/2\pi)\int \exp[i\gamma(sp+tq)]\Xi(s,t)\,ds\,dt.$$

It will be shown that the canonical Fourier–Plancherel transformation F is related to the Fourier–Plancherel–Weyl transformation by

$$F_\alpha = U_\gamma^{-1}(F\otimes F)\,U_\gamma$$

where $F\otimes F$ denotes the classical Fourier–Plancherel transformation on $L^2(\mathbb{R}^2)$,

$$F\otimes F\Xi(s,t) = (2\pi)^{-1}\int \exp[-i(ss'+tt')]\Xi(s',t')ds'\,dt',$$

and the parameters α and γ satisfy a certain relation.

A canonical analog has been formulated of the Wiener transformation,[4] which, in the case of one degree of freedom, is a unitary operator W_β acting in the Hilbert space H_β obtained by completing the space of formal polynomials in a canonical pair p and q with respect to the inner product

$$\langle X,Y\rangle = \omega_\beta(YX^*),$$

where for $X = \Sigma_{j,k} c_{j,k}p^j q^k$,

$$\omega_\beta(X) = \mathrm{tr}\sum_{j,k} c_{j,k}p_0^j q_0^k \rho_\beta,$$

$$\rho_\beta = \mathrm{tr}\exp[-\tfrac{1}{2}\beta(p_0^2+q_0^2)]\exp[-\tfrac{1}{2}\beta(p_0^2+q_0^2)]. \tag{1.2}$$

Here β is a fixed positive number. We shall show that if α and β are related in a certain way, then

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$$F_\alpha = V_\beta W_\beta V_\beta^{-1}, \tag{1.3}$$

where V_β is the unitary extension of the isometric map

$$\sum_{j,k} c_{j,k} p^j q^k \mapsto \sum_{j,k} c_{j,k} p_0^j q_0^k \rho_\beta^{1/2}$$

to H_β and F_α is taken to map $L^2(p_0,q_0)$ to itself. Thus for suitably related α, β, and γ, the diagram

$$\begin{array}{ccc} L^2(\mathbb{R}^2) & \xrightarrow{F\otimes F} & L^2(\mathbb{R}^2) \\ \uparrow U_\gamma & & U_\gamma^{-1}\downarrow \\ L^2(p_0,q_0) & \xrightarrow[F_\alpha]{} & L^2(p_0,q_0) \\ \downarrow V_\beta^{-1} & & V_\beta\uparrow \\ H_\beta & \xrightarrow[W_\beta]{} & H_\beta \end{array}$$

commutes. The relation (1.3) is an analog of the classical relation

$$F = M_d^{-1} W M_d, \qquad \text{where } d = \left(\frac{d\gamma}{dx}\right)^{1/2},$$

between the Fourier–Plancherel transformation F on $L^2(\mathbb{R})$, the classical one-dimensional Wiener transformation W, and the isometry M_d from $L^2(\mathbb{R},d\gamma)$ onto $L^2(R)$ which consists of multiplication by the square root of the density $d\gamma/dx$ of the normal distribution $d\gamma$ on R. In this connection, the nonexistence of an infinite-dimensional analog of Lebesgue measure which forces the replacement of the Fourier–Plancherel by the Wiener transformation in infinite-dimensional spaces has its analog in the fact that the representations of the canonical commutation relations associated with the infinite-degree-of-freedom analog of the states ω_β (extremal universally invariant states[5]) generate type III factors which possess no nontrivial traces and which therefore cannot support a Fourier–Plancherel type transformation. By contrast the canonical Wiener transformation, like its classical counterpart, can still be defined.[6]

2. THE CANONICAL FOURIER–PLANCHEREL TRANSFORMATION

Let N be a type I factor with faithful normal semi-finite trace τ. Let $N\otimes N$ be the von Neumann algebra tensor product of N with itself, which is also a type I factor equipped with the trace $\tau\otimes\tau$ for which $\tau\otimes\tau(X\otimes Y)=\tau(X)\tau(Y)$. Denote by N_* the class of traceable elements of N (which is canonically isomorphic to the predual of N). Fix $X\in N_*$ and $K\in N\otimes N$. For arbitrary $Y\otimes N_*$, $X\otimes Y$ is a traceable element of $N\otimes N$ and, since the traceable elements form an ideal, so also is $K(X\otimes Y)$. Moreover,

$$\begin{aligned} |(\tau\otimes\tau)(K(X\otimes Y))| &\leqslant \|K\|(\tau\otimes\tau)|X\otimes Y| \\ &= \|K\|(\tau\otimes\tau)|X|\otimes|Y| \\ &= \|K\|\tau(|X|)\tau(|Y|). \end{aligned}$$

Hence $Y\mapsto(\tau\otimes\tau)(K(X\otimes Y))$ is a bounded linear functional on the Banach space N_*, and so there exists an element $Z\in N$ such that

$$(\tau\otimes\tau)(K(X\otimes Y))=\tau(ZY).$$

We call Z the *partial trace* of $K(X\otimes 1)$.

Now let $N=N(p,q)$ be generated by a canonical pair p and q satisfying (1.1). We wish to define the unitary operator $\exp[i\alpha(p\otimes p+q\otimes q)]$ for real α. We recall that the Fourier–Plancherel transformation F in $L^2(\mathbb{R})$ intertwines the Schrödinger operators:

$$Fp_0F^{-1}=q_0, \qquad Fq_0F^{-1}=-p_0. \tag{2.1}$$

Hence, formally,

$$(1\otimes F)(p_0\otimes p_0+q_0\otimes q_0)(1\otimes F^{-1})=p_0\otimes q_0-q_0\otimes p_0.$$

By identifying $L^2(\mathbb{R})\otimes L^2(\mathbb{R})$ with $L^2(\mathbb{R}^2)$, the latter "angular momentum" operator can be defined rigorously as the infinitesimal generator of the coordinate rotations in $L^2(\mathbb{R}^2)$, so that $\exp[i\alpha(p_0\otimes q_0-q_0\otimes p_0)]$ acts on $f\in L^2(\mathbb{R}^2)$ as

$$\begin{aligned} &\exp[i\alpha(p_0\otimes q_0-q_0\otimes p_0)]f(s,t) \\ &\quad = f(\cos\alpha\, s+\sin\alpha\, t,-\sin\alpha\, s+\cos\alpha\, t). \end{aligned} \tag{2.2}$$

We now define $e^{[i\alpha(p\otimes p+q\otimes q)]}$ as

$$\begin{aligned} &e^{[i\alpha(p\otimes p+q\otimes q)]} \\ &\quad = (\nu\otimes\nu)^{-1}(1\otimes F)^{-1}\exp[i\alpha(p_0\otimes q_0-q_0\otimes p_0)](1\otimes F), \end{aligned}$$

where ν is the canonical isomorphism from $N(p,q)$ onto $B(L^2(\mathbb{R}))$.

Now let α be a fixed real number in the interval $(0,\pi)$. For $X\in N_*=N_*(p,q)$ we define the *Fourier transform* $\hat{X}\in N$ as the partial trace of $\sin\alpha\, e^{-i\alpha(p\otimes p+q\otimes q)}X\otimes 1$. [The normalization factor $\sin\alpha$ is convenient if the trace in $N(p,q)$ is normalized so as to transform into the standard trace on $B(L^2(R))$ under the canonical isomorphism, as we shall assume to be the case.] Similarly, we define the *inverse Fourier transform* $\check{X}$ of X as the partial trace of $\sin\alpha\, e^{i\alpha(p\otimes p+q\otimes q)}X\otimes 1$.

We observe that

$$\|\hat{X}\|\leqslant\|X\|_1, \quad \|\check{X}\|\leqslant\|X\|_1, \tag{2.3}$$

where $\|\ \|_1$ is the trace norm in $N_*(p,q)$.

We denote by $S(p,q)$ the space of elements of $N(p,q)$ which are pre-images under the canonical isomorphism ν of Hilbert–Schmidt operators in $B(L^2(\mathbb{R}))$ whose kernels (as integral operators) lie in the Schwarz space $S(\mathbb{R}^2)$ of infinitely differentiable rapidly decreasing functions on $\mathbb{R}$. If for $X\in S(p,q)$, νX has kernel $\xi\in S(\mathbb{R}^2)$ then $X\in N_*(p,q)$ and $\tau(X)$ is given by

$$\tau(X)=\int \xi(t,t)\,dt.$$

We shall prove that the mapping $X\to\hat{X}$ maps $S(p,q)$ isometrically (in the sense of the L^2 trace norm) onto itself and that its inverse maps $X\in S(p,q)$ to its inverse Fourier transform $\check{X}$. Since $S(p,q)$ is dense in $L^2(p,q)$ [because $S(\mathbb{R}^2)$ is dense in $L^2(\mathbb{R}^2)$], the Fourier transform mapping on $S(p,q)$ can thus be extended uniquely to an isometry F_α from $L^2(p,q)$ onto itself whose inverse is an extension of the inverse Fourier transform mapping on $S(p,q)$. By the boundedness relations (2.3) and the facts that convergence in the trace norm in $N_*(p,q)$ implies convergence in L^2 norm and that convergence in L^2 norm implies convergence in operator bound norm, it is clear that F_α and its inverse map arbitrary elements of $N_*(p,q)$ into their Fourier and inverse Fourier

transforms respectively. Thus we shall have proved the following Theorem.

Theorem 1: The mapping from $N(p,q)$ into $N(p,q)$ $X\to\hat{X}$, where $\hat{X}$ is the Fourier transform of X,

$$\hat{X}=\sin\alpha\ \tau_1 e^{-i\alpha(p\otimes p+q\otimes q)}X\otimes 1$$

extends uniquely to an isometry F_α from $L^2(p,q)$ onto itself, the restriction of whose inverse to $N_*(p,q)$ is the mapping $X\to\check{X}$, where $\check{X}$ is the inverse Fourier transform of X,

$$\check{X}=\sin\alpha\ \tau_1 e^{i\alpha(p\otimes p+q\otimes q)}X\otimes 1.$$

Proof: It is convenient to identify p and q with the Schrödinger canonical pair. Thus, let $X\in S(p,q)=S(p_0,q_0)$ have kernel $\xi\in S(\mathbb{R}^2)$, so that, for $f\in L^2(\mathbb{R})$,

$$Xf(s)=\int \xi(s,t)f(t)dt.$$

For $f, g\in L^2(\mathbb{R})$, we denote by g^*f the operator $h\mapsto\langle g,h\rangle f$. Then we have, for arbitrary $f, g\in S(\mathbb{R})$,

$$\begin{aligned}\langle g,\hat{X}f\rangle&=\mathrm{tr}\hat{X}g^*f\\&=\sin\alpha\ \mathrm{trexp}[-i\alpha(p_0\otimes p_0+q_0\otimes q_0)]X\otimes g^*f\\&=\sin\alpha\ \mathrm{tr}(1\otimes F)^{-1}\exp[-i\alpha(p_0\otimes q_0-q_0\otimes p_0)]\\&\quad(1\otimes F)X\otimes g^*f,\end{aligned}\tag{2.4}$$

where tr denotes the standard trace in $B(L^2(\mathbb{R}))$. Now $X\otimes g^*f$ is the integral operator in $L^2(\mathbb{R}^2)=L^2(\mathbb{R})\otimes L^2(\mathbb{R})$ whose kernel is

$$\xi_1(s_1,s_2,t_1,t_2)=\xi(s_1,t_1)f(s_2)\overline{g(t_2)}\ .$$

It is clear that $\xi_1\in S(\mathbb{R}^4)$. From this it follows successively that the kernel of $1\otimes FX\otimes g^*f$ is

$$\xi_2(s_1,s_2,t_1,t_2)=\xi(s_1,t_1)\hat{f}(s_2)\overline{g(t_2)}\ ,$$

where $\hat{f}$ is the Fourier transform of f, the kernel of $\exp[-i\alpha(p_0\otimes q_0-q_0\otimes p_0)](1\otimes F)X\otimes g^*f$ is

$$\begin{aligned}&\xi_3(s_1,s_2,t_1,t_2)\\&=\xi(\cos\alpha\ s_1-\sin\alpha\ s_2,t_1)\\&\quad\times\hat{f}(\sin\alpha\ s_1+\cos\alpha\ s_2)\overline{g(t_2)}\end{aligned}$$

[making use of (2.2)], and that the kernel of $(1\otimes F)^{-1}\exp[-i\alpha(p_0\otimes q_0-q_0\otimes p_0)](1\otimes F)X\otimes g^*f$ is given by

$$\xi_4(s_1,s_2,t_1,t_2)(1/\sqrt{2\pi}\,)\int\exp(is_2s'_2)\xi_3(s_1,s'_2,t_1,t_2)\ ds'_1.$$

Moreover, each kernel belongs to $S(\mathbb{R}^4)$. Since in particular $\xi_4\in S(\mathbb{R}^4)$, it follows that the trace in (2.4) can be evaluated as

$$\begin{aligned}&\int\xi_4(s_1,s_2,s_1,s_2)ds_1\,ds_2\\&=1/\sqrt{2\pi}\int\int\int\exp(is_2s'_2)\xi_3(s_1,s'_2,s_1,s_2)\,ds'_2ds_1\,ds_2\\&=1/\sqrt{2\pi}\int\int\int\exp(is_2s'_2)\xi_3(s_1,s'_2,s_1,s_2)ds_2ds'_2\,ds\\&=\int\int\xi(\cos\alpha\ s_1-\sin\alpha\ s'_2,s_1,)\hat{f}(\sin\alpha\ s_1\\&\quad+\cos\alpha\ s'_2)\ \overline{g(s'_2)}\ ds_2\,ds'_1,\end{aligned}$$

the change in order of integration being justified since the integrand is in $S(\mathbb{R}^3)$. Making the change of variables

$$t=\sin\alpha\ s_1+\cos\alpha\ s'_2,\quad s=-s'_2,$$

we obtain

$$\begin{aligned}&\langle g,\hat{X}f\rangle\\&=\int\int\xi(\cot\alpha t+\csc\alpha s,\csc\alpha t+\cot\alpha s)\hat{f}(t)\overline{\hat{g}(-s)}\ ds\,dt\\&=\int\int_{R_{M(\alpha)}}\xi(s,t)\hat{f}(t)\,\overline{\hat{g}(-s)}\,ds\,dt,\end{aligned}\tag{2.5}$$

where, for a real 2×2 matrix M, R_M is the operator in $L^2(\mathbb{R}^2)$

$$R_Mf(s,t)=f((s,t)M)$$

and $M(\alpha)$ is the matrix

$$M(\alpha)=\begin{pmatrix}\csc\alpha & \cot\alpha\\ \cot\alpha & \csc\alpha\end{pmatrix}.$$

Using the Plancherel identity in $L^2(\mathbb{R}^2)$, the relations

$$F\otimes F\ R_M=R_{(M')^{-1}}F\otimes F\tag{2.6}$$

$$\bar{\hat{g}}=\hat{\tilde{g}},$$

where $\tilde{g}(s)=\bar{g}(-s)$, and the fact that $M(\alpha)'=M(\alpha)$, we write (2.4) as

$$\langle g,\hat{X}f\rangle=\int\int_{R_{M(\alpha)^{-1}}}F\otimes F\xi(s,t)f(t)\bar{g}(s)ds\,dt.$$

This being the case of arbitrary f and $g\in s(\mathbb{R})$ shows that the bounded operator $\hat{X}$ is the Hilbert–Schmidt operator whose kernel is

$$\hat{\xi}=R_{M(\alpha)^{-1}}F\otimes F\xi.\tag{2.7}$$

Since both $F\otimes F$ and $R_{M(\alpha)^{-1}}$ are isometries in $L^2(\mathbb{R}^2)$ mapping $S(\mathbb{R}^2)$ onto itself, we deduce that the mapping $X\to\hat{X}$ maps $S(p,q)$ isometrically onto itself in the sense of the L^2 norm, as claimed.

Our argument is applicable to the mapping $X\to\check{X}$ by replacing α by $-\alpha$; in particular if X has kernel $\xi\in S(\mathbb{R}^2)$, $\check{X}$ has kernel

$$\check{\xi}=R_{M(-\alpha)^{-1}}F\otimes F\xi.$$

Hence the kernel of $\check{\hat{X}}$ is given by

$$\begin{aligned}&R_{M(-\alpha)^{-1}}F\otimes F\ R_{M(\alpha)^{-1}}F\otimes F\xi\\&=F\otimes F\ R_{M(-\alpha)}R_{M(\alpha)^{-1}}F\otimes F\xi\\&=F\otimes FR_{-I}F\otimes F\xi\\&=(F\otimes F)^{-1}F\otimes F\xi\\&=\xi,\end{aligned}$$

where we make use of the relations (2.6),

$$M(-\alpha)=-M(\alpha),$$

and

$$F\otimes FR_{-I}=(F\otimes F)^{-1}.$$

A similar argument shows that $\overset{\vee}{X}'X$ and the theorem is proved.

The isometry F_α is called the (*canonical*) *Fourier–Plancherel transformation.*

3. THE CONNECTION WITH THE FOURIER–PLANCHEREL–WEYL TRANSFORMATION

For $X\in N_\bullet(p,q)$ the *Fourier–Weyl transform*

$$\Xi(s,t)=(\gamma/\sqrt{2\pi})\tau e^{-i\gamma(sp+tq)}X \tag{3.1}$$

(where γ is a fixed nonzero real number) is a well-defined bounded continuous function on $\mathbb{R}^2$. [Boundedness follows from the inequality

$$\|\Xi\|\equiv\sup_{s,t\in\mathbf{R}}|\Xi(s,t)|=\sup_{s,t\in\mathbf{R}}\left|\frac{\gamma}{\sqrt{2\pi}}\tau e^{-i\gamma(sp+tq)}X\right|$$

$$\leqslant\sup_{s,t\in\mathbf{R}}\frac{|\gamma|}{\sqrt{2\pi}}\|e^{-i\gamma(sp+tq)}\|\tau(|X|)$$

$$=\frac{|\gamma|}{\sqrt{2\pi}}\|X\|_1,$$

and continuity is easily deduced from the strong continuity of the operator-valued function on $\mathbb{R}$

$$(s,t)\to\exp[-i\gamma(sp+tq)]=\exp[(-i\tfrac{1}{2}\gamma^2st)\times\exp(-i\gamma sp)\exp-i\gamma tq).]$$

We identify p and q with the Schrödinger canonical pair and consider $X\in S(p,q)=S(p_0,q_0)$ having kernel $\xi\in S(\mathbb{R}^2)$. Using the action in $L^2(\mathbb{R})$ of $\exp[-i\gamma(sp_0+tq_0)]$,

$$\exp[-i\gamma(sp_0+tq_0)]f(u)|=\exp[-i\gamma t(u-\tfrac{1}{2}\gamma s]f(u-\gamma s), \tag{3.2}$$

the kernel of $\exp[-i\gamma(sp+tq)]X$ is found to be

$$\xi_1(u,v)=\exp[-i\gamma t(u-\tfrac{1}{2}\gamma s)]\xi(u-\gamma s,v).$$

Since $\xi_1\in S(\mathbb{R}^2)$ the trace of this operator can be evaluated as

$$\int\xi_1(u,u)du=\int\exp[-i\gamma t(u-\tfrac{1}{2}\gamma s)]\xi(u-\gamma s,u)du$$

$$=\gamma^{-1}\int e^{-itu'}\xi(\gamma^{-1}u'-\tfrac{1}{2}\gamma s,\gamma^{-1}u'+\tfrac{1}{2}s)du',$$

making the substitution $u'=\gamma(u-\frac{1}{2}\gamma s)$. Hence the Fourier–Plancherel–Weyl transform of X is given by

$$\Xi=(1\otimes F)R_{K(\gamma)}\xi, \tag{3.3}$$

where $K(\gamma)$ is the matrix

$$K(\gamma)=\begin{pmatrix}-\frac{1}{2}\gamma & \frac{1}{2}\gamma\\ \gamma^{-1} & \gamma^{-1}\end{pmatrix}.$$

Since $1\otimes F$ and $R_{K(\gamma)}$ are both isometries from $L^2(\mathbb{R}^2)$ onto itself leaving $S(\mathbb{R}^2)$ invariant, the Fourier–Weyl transform mapping maps $S(p,q)$ isometrically onto $S(\mathbb{R}^2)$ in the sense of the respective L^2 norms. Moreover, its inverse maps an element $\Xi\in S(\mathbb{R}^2)$ into the Hilbert–Schmidt operator with kernel

$$\xi(s,t)=R_{K(\gamma)^{-1}}(1\otimes F)^{-1}\Xi(s,t).$$

It may be verified using (3.2) that this is the operator-valued integral

$$X=(\gamma/\sqrt{2\pi})\int\exp[-i\gamma(sp_0+tq_0)]\Xi(s,t)dsdt,$$

but we shall make no use of this.

The *Fourier–Plancherel–Weyl transformation* U_γ is the unique isometry from $L^2(p,q)$ onto $L^2(\mathbb{R}^2)$ which extends the map $S(p,q)\ni X\to\Xi$, where Ξ is given by (3.3). It may then be shown that U_γ maps arbitrary $X\in N_\bullet(p,q)$ according to (3.1), and that its inverse acts on arbitrary $\Xi\in L^2(\mathbb{R})\cap L^1(\mathbb{R}^2)$ according to (3.4).[7,8]

Let us now consider the map $U_\gamma^{-1}(F\otimes F)U_\gamma$ from $S(p,q)$ to itself. If X has kernel ξ, then, using (3.3) we see that $U_\gamma^{-1}(F\otimes F)U_\gamma X$ has kernel

$$R_{K(\gamma)^{-1}}(1\otimes F)^{-1}(F\otimes F)(1\otimes F)R_{K(\gamma)}\xi$$
$$=R_{K(\gamma)^{-1}}F\otimes FR_{K(\gamma)}\xi$$
$$=R_{K(\gamma)^{-1}}R_{(K(\gamma)')^{-1}}F\otimes F\xi$$
$$=R_{(K(\gamma)'K(\gamma))^{-1}}F\otimes F,$$

using (2.5). Evaluating the matrix $(K(\gamma)'K(\gamma))^{-1}$ as

$$(K(\gamma)'K(\gamma))^{-1}=\begin{pmatrix}\gamma^{-2}+\frac{1}{4}\gamma^2 & -\gamma^{-2}+\frac{1}{4}\gamma^2\\ -\gamma^2+\frac{1}{4}\gamma^2 & \gamma^{-2}+\frac{1}{4}\gamma^2\end{pmatrix}$$

and comparing with (2.7), we see that the operator $U^{-1}(F\otimes F)UX$ coincides wih $F_\alpha X$ for all $X\in S(p,q)$, and hence for all $X\in L^2(p,q)$, provided that

$$\csc\alpha=\gamma^{-2}+\tfrac{1}{4}\gamma^2,\qquad\cot\alpha=\gamma^{-2}-\tfrac{1}{4}\gamma^2,$$

that is,

$$\alpha=\begin{cases}2\tan^{-1}(\frac{1}{2}\gamma^2) & (\gamma^2\leqslant 2)\\ 2\tan^{-1}(2\gamma^2) & (\gamma^2>2)\end{cases}. \tag{3.5}$$

We have proved the following:

Theorem 2: Provided that the parameters α and γ are related by (3.5), the canonical Fourier–Plancherel transformation F_α, the Fourier–Plancherel–Weyl transformation U_γ, and the Fourier–Plancherel transformation $F\otimes F$ on $L^2(\mathbb{R}^2)$ satisfy

$$F_\alpha=U_\gamma^{-1}(F\otimes F)U_\gamma.$$

4. THE CONNECTION WITH THE CANONICAL WIENER TRANSFORMATION

A canonical analog of the Wiener transformation[9,10] has been formulated,[11] which, in the case of one degree of freedom, assumes the following form. Consider the *Weyl algebra* $\mathscr{A}$ of formal polynomials in elements p and q satisfying the Heisenberg commutation relation

$$pq-qp=-i. \tag{4.1}$$

Equip $\mathscr{A}$ with the involution * for which $p=p^*$ and $q=q^*$. The map $p^m q^n \to p_0^m q_0^n$, where p_0 and q_0 are the Schrödinger canonical pair and $p_0^m q_0^n$ has domain $S(R)$, extends to a representation π_0 of $(\mathscr{A},*)$ in the sense of Powers,[12] and the formula

$$\omega_\beta(A)=\mathrm{tr}\pi_0(A)\rho_\beta$$

where β is a fixed positive number and ρ_β is given by (1.2), defines a state ω_β of $(\mathscr{A},*)$ analogous to a normal distribution.[13] It can be shown[14] that $\pi_0(A)\rho_\beta$ is traceable. Since the elements $\sqrt{2}p\otimes 1 \mp i1\otimes p$ and $\sqrt{2}\otimes 1 \mp i1\otimes q$ of the algebraic tensor product $\mathscr{A}\otimes\mathscr{A}$ satisfy (4.1), there are unique isomorphisms $\eta_\mp$ from $\mathscr{A}$ into $\mathscr{A}\otimes\mathscr{A}$ which map p and q into these elements. We may abuse notation by writing $A(\sqrt{2}p\otimes 1\mp 1\otimes p,\ \sqrt{2}q\otimes 1\mp i1\otimes q)$ for the image of $A=A(p,q)$, under $\eta_\mp$. The *Wiener transform* of an element $A\in\mathscr{A}$ is the element $\tilde{A}=\omega_{\beta,1}\eta_- A$, where $\omega_{\beta,1}$ is the linear mapping from $\mathscr{A}\otimes\mathscr{A}$ to $\mathscr{A}$ for which $\omega_{\beta,1}(A\otimes B)=\omega_\beta(A)B$. Formally

$$\tilde{A}(p,q)=\mathrm{tr}_{p_0,q_0}A(\sqrt{2}p_0-ip,\ \sqrt{2}q_0-iq)\rho_\beta.$$

It can be shown[15] that the mapping $A\to\tilde{A}$ is bijective on $\mathscr{A}$ and isometric in the inner product $\langle A,B\rangle=\omega_\beta(BA^*)$, and hence extends uniquely to a unitary operator W_β, the *canonical Wiener transformation* on the completion H_β of the inner product space $\mathscr{A}$. The inverse Wiener transformation acts on $\mathscr{A}$ as $\omega_{\beta,1}\eta_+$, so that formally,

$$W_\beta^{-1}A(p,q)=\mathrm{tr}_{p_0,q_0}A(\sqrt{2}p_0+ip,\sqrt{2}q_0+iq)\rho_\beta.$$

It can be shown[16] that the mapping $\mathscr{A}\ni A\to\pi_0(A)\Omega_\beta$, where $\Omega_\beta=\rho_\beta^{1/2}$, extends uniquely to an isometry V_β from H_β onto the Hilbert space $L^2(p_0,q_0)$ of Hilbert-Schmidt operators on $L^2(\mathbb{R})$.

Theorem 3: If

$$\tan\alpha=\sinh(\tfrac{1}{2}\beta), \tag{4.2}$$

then

$$F_\alpha=V_\beta W_\beta V_\beta^{-1}.$$

Proof: We introduce elements $H_{m,n}$ of $\mathscr{A}$, analogous to Hermite polynomials, by means of the generating function

$$G(u,v)=\exp[i(up+vq)+\tfrac{1}{4}\sigma^2(u^2+v^2)]=\sum_{m,n=0}^{\infty}H_{m,n}u^m v^n,$$

where

$$\sigma^2=\coth(\tfrac{1}{2}\beta)=\csc\alpha \tag{4.3}$$

{so that[17]

$$\mathrm{tr}\exp[i(up_0+vq_0)]\rho_\beta=\exp[-\tfrac{1}{4}\sigma^2(u^2+v^2)]\}. \tag{4.4}$$

The Wiener transforms of the elements $H_{m,n}$ are found from the formal calculation

$$W_\beta G(u,v)$$

$$=\mathrm{tr}_{p_0,q_0}\exp\{i[u(\sqrt{2}p_0-ip)+v(\sqrt{2}q_0-iq)+\tfrac{1}{4}\sigma^2(u^2+v^2)]\}$$

$$=\{\mathrm{tr}_{p_0,q_0}\exp[i(\sqrt{2}up_0+\sqrt{2}vq_0)]\rho_\beta\}\times\exp[up+vq+\tfrac{1}{4}\sigma^2(u^2+v^2)]$$

$$=\exp[up+vq-\tfrac{1}{4}\sigma^2(u^2+v^2)]=G(-iu,-iv)$$

using (4.4). From this it follows that

$$W_\beta H_{m,n}=(-i)^{m+n}H_{m,n}. \tag{4.5}$$

Now let $h_{m,n}$ be the image of $H_{m,n}$ under V_β. We show that the $h_{m,n}$ are eigenvectors of F_α with eigenvalues $(-i)^{m+n}$. We introduce the generating function

$$g(u,v)=\sum_{m,n=0}^{\infty}h_{m,n}u^m v^n$$

$$=\exp[i(up_0+vq_0)+\tfrac{1}{4}\sigma^2(u^2+v^2)]\Omega_\beta.$$

Now the kernel ζ_0 of the operator Ω_β is given[4] by

$$\zeta_0(s,t)=\pi^{-1/2}\exp[-\tfrac{1}{2}\coth(\tfrac{1}{2}\beta)(s^2+t^2)+\mathrm{csch}(\tfrac{1}{2}\beta)st]$$

$$=\pi^{-1/2}\exp\left[-\tfrac{1}{2}(s,t)M(\alpha)^{-1}\begin{pmatrix}s\\t\end{pmatrix}\right],$$

using (4.2). Using the action of $\exp[i(up_0+vq_0)]$,

$$\exp[i(up_0+vq_0)]f(s)=\exp[iv(s+\tfrac{1}{2}u)]f(s+u),$$

we deduce that the kernel of $g(u,v)$ is given by

$$\zeta(s,t;u,v)=\exp[\tfrac{1}{4}\sigma^2(u^2+v^2)]\exp[iv(s+\tfrac{1}{2}u)]$$

$$=\exp[\tfrac{1}{4}\sigma^2(-u+v^2)+\tfrac{1}{2}iuv] \tag{4.6}$$

$$\times\exp[ivs+u(\csc\alpha\, s-\cot\alpha\, t)]$$

$$\times\exp\left[-\tfrac{1}{2}(s,t)M(\alpha)^{-1}\begin{pmatrix}s\\t\end{pmatrix}\right] \tag{4.7}$$

using (4.2) and (4.3). Since this kernel is in $S(\mathbb{R}^2)$, we may apply (2.7) to (4.6) to obtain that the kernel of $F_\alpha\, g(u,v)$ is given by

$$\zeta(s,t;u,v)=\exp[\tfrac{1}{4}\sigma^2(u^2+v^2)]$$

$$\times\exp[-iu((\csc\alpha\, s-\cot\alpha\, t)+\tfrac{1}{2}v)]$$

$$\times R_{M(\alpha)^{-1}}F\otimes F\zeta_0(s-v,t)\ .$$

Now the Fourier transform of the quadratic exponential

$$\zeta_0(s,t)=\pi^{-1/2}\,e\,\mathrm{xp}\left[-\tfrac{1}{2}(s,t)M(\alpha)^{-1}\begin{pmatrix}s\\t\end{pmatrix}\right]$$

is obtained by inverting the matrix of the quadratic form; thus

$$F\otimes F\zeta_0(s,t)=\pi^{-1/2}\exp\left[-\tfrac{1}{2}(s,t)M(\alpha)\begin{pmatrix}s\\t\end{pmatrix}\right].$$

From this we see that

$$R_{M(\alpha)^{-1}}F\otimes F\zeta_0(s,t)$$

$$=\pi^{-1/2}\exp\left[-\tfrac{1}{2}(s,t)M(\alpha)^{-1}M(\alpha)(M(\alpha)^{-1})^t\begin{pmatrix}s\\t\end{pmatrix}\right]$$

$$=\zeta_0(s,t)$$

(Thus Ω_β is its own canonical Fourier transform.) Using this fact together with (4.3), we obtain

$$\begin{aligned}\hat{\zeta}(s,t;u,v) &= \exp[\tfrac{1}{4}\sigma^2(u^2-v^2)-\tfrac{1}{2}iuv] \\ &\quad\times\exp[vt-iu(\csc\alpha\, s-\cot\alpha\, t)] \\ &\quad\times\pi^{-1/2}\exp[-\tfrac{1}{2}(s,t)M(\alpha)^{-1}\begin{pmatrix}s\\t\end{pmatrix}] \\ &= \zeta(s,t;-iu,-iv) \qquad (4.8)\end{aligned}$$

by comparison with (4.7). From (4.8) we obtain that $F_\alpha g(u,v)=g(-iu,-iv)$ and hence that

$$F_\alpha h_{m,n}=(-i)^{m+n}h_{m,n} \qquad (4.9)$$

as claimed.

Comparing (4.5) with (4.8) and recalling that $h_{m,n}=V_\beta H_{m,n}$, we see that the unitary operators W_β and $V_\beta^{-1}F_\alpha V_\beta$ in H_β both have the elements $H_{m,n}$ as eigenvectors, with the same eigenvalues $(-i)^{m+n}$. Now inspection of the generating function $G(u,v)$ shows that $H_{m,n}$ is of the form

$$H_{m,n}=i^{m+n}(m!n!)^{-1}p^m q^n+J_{m,n},$$

where $J_{m,n}$ is a polynomial in p and q of degree less than $m+n$. It follows that the elements $H_{m,n}$ span the space $\mathscr{A}$. Hence the unitary operators W_β and $V_\beta^{-1}F_\alpha V_\beta$ possess a total set of eigenvectors on which they have the same eigenvalues. Hence they are coincident. From this it follows that $F_\alpha=V_\beta W_\beta V_\beta^{-1}$, and the theorem is proved.

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Colliding plane gravitational waves

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New exact solutions of the vacuum Einstein field equations are constructed which describe the collision of plane gravitational waves. These solutions generalize those of Szekeres by relaxing the requirement of collinear polarization.

I. INTRODUCTION

Penrose[1] discovered that in the field of plane gravitational waves null rays are focused on certain hypersurfaces where the Riemann tensor takes divergent values. Another situation where such focusing effects appear explicitly is the collision of two gravitational plane waves where each wave is focused by the field of the other and the resulting configuration possesses a space–time singularity. All these properties are verified by the exact solutions of Einstein equations given by Khan and Penrose[2] for colliding impulsive waves and Szekeres[3,4] for shock waves. These solutions, describing the collision between plane gravitational waves with constant linear polarization enable us to study the details of this focusing. It is natural to ask how the focusing properties and the resulting space–time singularity are modified when we introduce new degrees of freedom into the problem. For this purpose we have recently presented a new solution of the vacuum Einstein field equations which describes colliding impulsive gravitational waves with linear but not necessarily collinear polarizations.[5] This implies that the colliding plane waves are still linearly polarized but their directions of polarization are out of phase by a constant phase parameter. We have pointed out that certain features of the problem are modified; for example, the collision results in giving an angular momentum as well as a mass aspect to the gravitational field in the interaction region. The physical space–time singularity on the other hand, although undergoing minor modifications by this additional degree of freedom, is still present. Furthermore Szekeres' conclusion that the space–time singularities arise inevitably for arbitrarily weak incoming gravitational waves remains valid in this new situation as well. The general problem which takes into account the effect of arbitrary polarization has been considered by Sbytov[6] who showed without giving explicit solutions that the physical singularity appears even when the effect of arbitrary polarization is taken into account. The singularity in these solutions of Einstein's equations results from the assumptions of planar wave fronts as pointed out by Penrose[1] a long time ago.

In this paper we shall present a family of exact solutions which generalizes the family of Szekeres to the case of non-collinear polarizations. The first member of this family (i.e., impulsive waves) has already been given in Ref. 5. The plan for this paper is as follows: In Sec. II we shall review the Szekeres' solutions and cast them into a form where the colliding waves initially have a constant phase difference between them. Our method for obtaining the new solutions is based on the theory of harmonic mappings of Riemannian manifolds due to Eells and Sampson.[7] The application of this theory to general relativity[8–10] proved to be a useful technique that facilitates the solution of many problems. For the paper to be self-contained we shall briefly present the necessary tools for applying the theory of harmonic maps.

In Sec. III using harmonic maps we cast the basic field equations of this problem into a form similar to Ernst's[11] for axisymmetric fields. The solutions is then immediate, and we adapt a solution which involves two arbitrary constants. One of these constants which corresponds to the relative polarization angle of the incoming waves is an analog of Kerr's rotation parameter. The second constant on the other hand is a Taub–NUT like parameter which has no immediate physical interpretation for the colliding wave problem. Furthermore, there are other solutions of the field equations which include a Weyl–Tomimatsu–Sato parameter, but these solutions must be excluded as they do not reduce to the desired incoming and outgoing plane wave solutions. While in the family of Szekeres' solutions there are two independent parameters, we have been able to generalize them only for the case when these two parameters are equal. Finally in the Appendix we calculate the Newman–Penrose[12] curvature components which manifests the singularities of these solutions.

II. COLLIDING PLANE GRAVITATIONAL WAVES

Grvaitational plane waves are described by the metric for p-p waves[13]

$$ds^2=2du'dv'-dx'^2-dy'^2-2H(x',y',u')du'^2, \tag{1}$$

where $H(x',y',u')$ is the real part of an analytic function in $x'+iy'$ and an arbitrary function of u'. For plane waves with constant linear polarization $H(x',y',u')$ takes the form

$$H(x',y',u')=h(u')(y'^2-x'^2), \tag{2}$$

where $h(u')$ is given in the case of Szekeres' family of solutions by

$$h(u')=u'^{n-1}\delta(u') + \frac{n(1-n)(2-1/n)^{1/2}u(u')^{2(n-1)}\theta(u(u'))}{8(1-u^{2n}(u')\theta(u(u'))^2}, \tag{3}$$

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where u' is the harmonic coordinate appearing in the canonical form of the line element (1) while u is the Rosen coordinate whose relation to u' is given below. Here, θ denotes the Heaviside unit step function and the integer n satisfies the condition $n \geqslant 1$. We notice here that, for $n=1$, $h(u')=\delta(u')$ which corresponds to impulsive waves while for higher values of n it corresponds to shock waves. For discussing the problem of colliding waves it is necessary to obtain a C^0 form of the metric, we therefore transform to the Rosen form

$$ds^2=2e^{-M}dudv-e^{-U}[e^{V}\cosh W\,dx^2 + e^{-V}\cosh W\,dy^2 - 2\sinh W\,dxdy\ ], \tag{4}$$

where M, U, V, and W are functions of the null coordinates (u,v) only. For the case of Szekeres' family Rosen form is accomplished by the transformation

$$\begin{aligned} x' &= (1-u^n\theta)^{1/2-\kappa/2}(1+u^n\theta)^{1/2+\kappa/2}X, \\ y' &= (1+u^n\theta)^{1/2-\kappa/2}(1-u^n\theta)^{1/2+\kappa/2}Y, \\ u' &= \int_0^u (1-u^{2n}\theta)^{(1-1/n)/2}du, \\ v' &= v+\tfrac{1}{2}n\,u^{n-1}\theta(u)[1-u^{2n}\theta(u)]^{1/n-1/2} \\ &\quad\times\{X^2[\kappa-u^n\theta(u)][1+u^n\theta(u)]^{\kappa/2} \\ &\quad\times[1-u^n\theta(u)]^{-\kappa/2}-Y^2[\kappa+u^n\theta(u)] \\ &\quad\times[1+u^n\theta(u)]^{-\kappa/2}[1-u^n\theta(u)]^{\kappa/2}\}, \end{aligned} \tag{5}$$

where κ is a real parameter related to n by

$$\kappa^2=2-1/n \tag{6}$$

and the Rosen form of the metric is given as

$$\begin{aligned} ds^2 &= 2[1-u^{2n}\theta(u)]^{(1-1/n)/2}dudv-[1-u^{2n}\theta(u)] \\ &\quad\times\{[1-u^n\theta(u)]^{-\kappa}[1+u^n\theta(u)]^{\kappa}dX^2 \\ &\quad+[1+u^n\theta(u)]^{-\kappa}[1-u^n\theta(u)]^{\kappa}dY^2\}. \end{aligned} \tag{7}$$

The metric (4) represents the most general form for plane waves with arbitrary polarization. In the case of linear polarization we have the simplifying feature that $W=0$, but in this paper we shall investigate the collision of linearly polarized plane waves with a relative phase difference which require two mutually nonorthogonal Killing vectors ξ_x and ξ_y. So we shall now introduce a new parameter which measures the angle of polarization of the gravitational wave within the coordinate system under consideration. For convenience we choose this parameter to be the angle of rotation of (X,Y) coordinates in accordance with

$$X+iY = e^{i(\pi/2-\alpha\kappa)/2}(x+iy), \tag{8}$$

α being a real parameter. Now we obtain the metric (7) in the form

$$\begin{aligned} ds^2 &= 2(1-p^2)^{(1-1/n)/2}dudv-\frac{(1-p^2)}{2P} \\ &\quad\times\{[1+P^2+(1-P^2)\sin\alpha\kappa]dx^2 \\ &\quad+[1+P^2-(1-P^2)\sin\alpha\kappa]dy^2 \\ &\quad+2\cos\alpha\kappa(P^2-1)dxdy\}, \end{aligned}$$

where

$$P=\left(\frac{1-p}{1+p}\right)^{\kappa},\quad p=u^n\theta(u). \tag{9}$$

Let us note that with this choice of the rotation angle the choice $\alpha\kappa=\pi/2$ results in Eq. (7). In order to discuss collision of gravitational plane waves, it is convenient to consider space–time manifold in four disjoint patches as in Fig. 1. Let us consider two gravitational plane waves travelling in $+z$ and $-z$ directions. Prior to the collision of these waves the space–time region between them (region I) is Minkowski space while region II is given by the nonflat metric (9). We obtain region III from region II by replacing $u \leftrightarrow v$ and $\alpha \leftrightarrow \beta$ everywhere. In region II we shall employ the following null tetrad,

$$\begin{aligned} l_\mu &= (1-p^2)^{(1-1/n)/2}\delta_\mu{}^0, \\ n_\mu &= \delta_\mu{}^1, \\ m_\mu &= 2^{-1/2}[(1-p)^{(1-\kappa)/2}(1+p)^{(1+\kappa)/2}\delta_\mu{}^2 \\ &\quad+i(1+p)^{(1-\kappa)/2}(1-p)^{(1+\kappa)/2}\delta_\mu{}^3], \end{aligned} \tag{10}$$

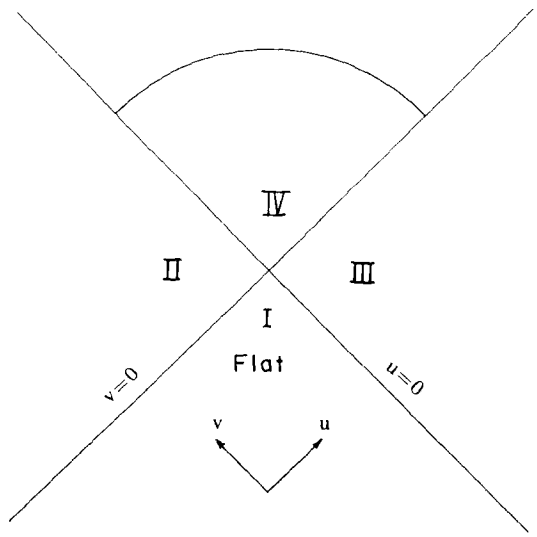

FIG. 1. Space–time diagram for colliding gravitational plane waves.

and we find that

$$\lambda = n\kappa u^{n-1}\theta(u)(1-p^2)^{(1/n-3)/2},$$

$$\mu = -n u^{2n-1}\theta(u)(1-p^2)^{(1/n-3)/2},$$

$$\psi_4 = \kappa n (1-p^2)^{1/n-3}[(1-n)u^{n-2} - u^{n-1}\delta(u)], \quad (11)$$

are the only nonvanishing Newman–Penrose (NP) quantities. The metric (7) represents a type N field. Similarly for the region III the nonvanishing NP quantities are σ, p, and ψ_0. We shall now consider the space–time geometry in the interaction region using these solutions as boundary conditions. The resulting space–time in the interaction region (region IV) becomes algebraically general.

The Einstein field equations for the metric (4) are well known, but as in Ref. 5 we shall use of Eells and Sampson's theory of harmonic mappings of Riemannian manifolds to cast the problem into a simple form. We consider two Riemannian manifolds (M,g) and (M',g') with dimensionalities n,n' respectively and a map $f: M \to M'$. Eells and Sampson's energy functional, which in local coordinates is given by

$$E(f) = \int g'_{AB} \frac{\partial f^A}{\partial x^i} \frac{\partial f^A}{\partial x^k} g^{ik} |g|^{1/2} d^n x, \quad (12)$$

defines an invariant functional of the mapping. We shall be interested in those maps for which the first variation vanishes

$$\delta E(f) = 0, \quad (13)$$

i.e., harmonic maps. We had shown earlier that the Einstein field equations for the metric (4) are obtained as harmonic maps where M is a flat two-dimensional manifold with the metric

$$ds^2 = 2du dv \quad (14)$$

and M' has metric

$$ds'^2 = e^{-U}(2dM\,dU + dU^2 - dW^2 - \cosh^2 W\, dV^2) \quad (15)$$

If we vary the energy functional formed from these two metrics, we obtain the Einstein field equations first obtained for this problem by Szekeres who used a different approach based on the Newman–Penrose formalism.

III. NEW FAMILY OF EXACT SOLUTIONS

We shall now derive a new family of exact solutions of the Einstein's field equations which correspond to the collision of linearly polarized plane gravitational waves with different phase parameters. These will generalize exact solutions for collinear polarizations given by Khan–Penrose and Szekeres. For this purpose we shall consider the metric for M' manifold. As we noted earlier the 2-section of this manifold spanned by V and W coordinates is a space of constant curvature, but in order to change this line element into the normal form we first imbed this 2-section in a three-dimensional flat manifold. The imbedding coordinates are given by

$$\alpha = \cosh V \cosh W + \sinh W,$$

$$\beta = \cosh V \cosh W - \sinh W,$$

$$\gamma = \sinh V \cosh W, \quad (16)$$

subject to the constraint

$$\alpha\beta - \gamma^2 = 1. \quad (17)$$

The relevant part of the metric becomes $d\alpha d\beta - d\gamma^2$. Now let us choose a new parametrization which satisfies the constraint Eq. (17) by letting

$$\alpha = \cos\nu \sinh\omega + \cosh\omega,$$

$$\beta = -\cos\nu \sinh\omega + \cosh\omega,$$

$$\gamma = \sin\nu \sinh\omega, \quad (18)$$

the metric of M' then takes the form

$$ds'^2 = e^{-U}(2dM\,dU + dU^2 - d\omega^2 - \sinh^2\omega\, d\nu^2), \quad (19)$$

which is the required form. Once we have cast the metric of M' into this form we introduce a complex function η which is defined by

$$\eta = e^{i\nu/\kappa}\tanh\frac{\omega}{2\kappa}, \quad (20)$$

where κ is a constant so that the metric of M' becomes

$$ds'^2 = e^{-U}\left(2dM\,dU + dU^2 - 4\kappa^2 \frac{d\eta d\bar{\eta}}{(1-\eta\bar{\eta})^2}\right), \quad (21)$$

where the bar denotes complex conjugation. Varying the energy functional constructed from the metrics (14) and (21) with respect to M, U, and $\bar{\eta}$, we get the field equations

$$(e^{-U})_{uv} = 0, \quad (22)$$

$$2M_{uv} + U_{uv} = 2\kappa^2(\eta_u\bar{\eta}_v + \eta_v\bar{\eta}_u)(\eta\bar{\eta} - 1)^{-1}, \quad (23)$$

$$2\eta_{uv} - U_v\eta_u - U_u\eta_v = 4\bar{\eta}\eta_u\eta_v(\eta\bar{\eta} - 1)^{-1}. \quad (24)$$

There is an analogy between Eq. (24) and the Einstein's equation for stationary axisymmetric gravitational fields in Ernst's formulation

$$(\xi\bar{\xi} - 1)\nabla^2\xi = 2\bar{\xi}\nabla\xi\cdot\nabla\xi. \quad (25)$$

Note, however, that the definition of η in Eq. (20) is entirely different from Ernst's ξ. The crucial point here is the following: We want the coupled partial differential equations to be a familar set of equations so that we can directly write their solutions, but the choice of dependent as well as independent variables are further restricted by the requirement that the resulting solution should have the proper boundary conditions. These considerations suggest that we search for a coordinate transformation so that we can pass from the patch $\{u,v\}$ to another patch $\{\tau,\sigma\}$ which has properties analogous to prolate spheroidal coordinates. This transformation is given by

$$\tau=u^{n}(1-v^{2n})^{1/2}+v^{n}(1-u^{2n})^{1/2},$$

$$\sigma=u^{n}(1-v^{2n})^{1/2}+v^{n}(1-u^{2n})^{1/2}, \tag{26}$$

where $n\geqslant 1$ is an integer. Under this change of coordinates the metric of M is transformed into

$$ds^2=\Omega(\tau,\sigma)\left(\frac{d\tau^2}{1-\tau^2}-\frac{d\sigma^2}{1-\sigma^2}\right), \tag{27}$$

where the conformal factor Ω is irrelevant because it does not enter into the energy functional in Eq. (12). The usefulness of these new coordinates will appear when we rewrite the differential operators in the field equations using the $\{\tau,\sigma\}$ coordinate patch. First we note that in region IV

$$e^{-U}=1-u^{2n}-v^{2n}=(1-\tau^2)^{1/2}(1-\sigma^2)^{1/2} \tag{28}$$

and two useful identifies are given by

$$2\psi_{uv}-U_v\psi_u-U_u\psi_v$$
$$=\Omega(\tau,\sigma)\{[(1-\tau^2)\psi_\tau]_\tau-[(1-\sigma^2)\psi_\sigma]_\sigma\}, \tag{29}$$

$$\psi_u\chi_v+\psi_v\chi_u$$
$$=\Omega(\tau,\sigma)\{(1-\tau^2)\psi_\tau\chi_\tau-(1-\sigma^2)\psi_\sigma\chi_\sigma\}, \tag{30}$$

where ψ and χ are any two functions which are at least twice differentiable. It is straightforward to show that Eq. (24) in the coordinate patch $\{\tau,\sigma\}$ is given by

$$(\eta\bar{\eta}-1)\{[(1-\tau^2)\eta_\tau]_\tau-[(1-\sigma^2)\eta_\sigma]_\sigma\}$$
$$=2\bar{\eta}\{(1-\tau^2)\eta_\tau^2-(1-\sigma^2)\eta_\sigma^2\}, \tag{31}$$

which is the familiar Ernst's equation. It is well known that it admits a solution of the form

$$\eta=e^{i[(\alpha+\beta)/2]}\left[\tau\cos\left(\frac{\alpha-\beta}{2}\right)+i\sigma\sin\left(\frac{\alpha-\beta}{2}\right)\right], \tag{32}$$

where the arbitrary constants α and β are chosen to be polarization parameters in regions II and III respectively. Taking into considerations the boundary effects of the different space–time regions, we let $u\to u\theta(u)$ and $v\to v\theta(v)$ so that the solution (32) is equivalent to

$$\eta=e^{i\alpha}pw+e^{i\beta}qr, \tag{33}$$

where

$$p=u^{n}\theta(u),\quad q=v^{n}\theta(v),\quad r^2=1-p^2,\quad w^2=1-q^2.$$

Comparing the solution (32) with that given by Ernst for axisymmetric gravitational fields we immediately notice that $(\alpha-\beta)/2$ plays the role of a rotation parameter while $(\alpha+\beta)/2$ is the Taub–NUT parameter. Using this solution in the $\{u,v\}$ patch [i.e., Eq. (33)], we shall proceed to construct the space–time metric and show that it has the correct boundary values. This amounts to the determination of M, U, V, and W. From the definition (20) and (33) we read the solutions for ω and ν,

$$\sin\frac{\nu}{\kappa}=\frac{1}{|\eta|}(pw\sin\alpha+qr\sin\beta), \tag{34}$$

$$\sinh\frac{\omega}{\kappa}=\frac{2|\eta|}{1-|\eta|^2}. \tag{35}$$

The original metric functions V and W are given in terms of ω and ν by

$$e^{2V}=\frac{\cos\omega+\sin\nu\sinh\omega}{\cosh\omega-\sin\nu\sinh\omega}, \tag{36}$$

$$\sinh W=\cos\nu\sinh\omega. \tag{37}$$

In order to determine M, we integrate (23), so that the final solution for the metric functions is given as follows

$$e^{-U}=t^2=1-p^2-q^2, \tag{38}$$

$$e^{-M}=t^{-1}(rw)^{-\kappa^2}(1-|\eta|^2)^{\kappa^2}, \tag{39}$$

$$\sinh W=\frac{\eta^\kappa+\bar{\eta}^\kappa}{4|\eta|^\kappa}\left[\left(\frac{1+|\eta|}{1-|\eta|}\right)^\kappa-\left(\frac{1-|\eta|}{1+|\eta|}\right)^\kappa\right], \tag{40}$$

$$e^{2V}=\frac{(1+|\eta|)^{2\kappa}(2i|\eta|^\kappa+\eta^\kappa-\bar{\eta}^\kappa)+(1-|\eta|)^{2\kappa}(2i|\eta|^\kappa-\eta^\kappa+\bar{\eta}^\kappa)}{(1+|\eta|)^{2\kappa}(2i|\eta|^\kappa-\eta^\kappa+\bar{\eta}^\kappa)+(1-|\eta|)^{2\kappa}(2i|\eta|^\kappa+\eta^\kappa-\bar{\eta}^\kappa)} \tag{41}$$

where n and κ are related by (6). This solution may be expressed in terms of a null tetrad defined as

$$l_\mu=e^{-M/2}\delta^0_\mu,$$

$$n_\mu=e^{-M/2}\delta^1_\mu,$$

$$m_\mu=\tfrac{1}{2}e^{-U/2}[e^{V/2}(i\sinh\tfrac{1}{2}W-\cosh\tfrac{1}{2}W)\delta^2_\mu+e^{-V/2}(\sinh\tfrac{1}{2}W-i\cosh\tfrac{1}{2}W)\delta^3_\mu]. \tag{42}$$

Now let us show that in the second region limit the solution (38)–(41) coincides with the Rosen form (9). For this purpose we set $q=0$ and obtain the solution

$$e^{-U}\equiv t^2=1-p^2, \tag{43}$$

$$e^{-M}=t^{\kappa^2-1}, \tag{44}$$

$$\sinh W=\tfrac{1}{2}\cos\alpha\kappa\left[\left(\frac{1+p}{1-p}\right)^{\kappa}-\left(\frac{1-p}{1+p}\right)^{\kappa}\right], \tag{45}$$

$$e^{2V}=\frac{(1+p)^{2\kappa}+(1-p)^{2\kappa}+\sin\alpha\kappa[(1+p)^{2\kappa}-(1-p)^{2\kappa}]}{(1+p)^{2\kappa}+(1-p)^{2\kappa}-\sin\alpha\kappa[(1+p)^{2\kappa}-(1-p)^{2\kappa}]}, \tag{46}$$

which gives the metric (9) so that the boundary conditions are satisfied. For $n=\kappa=1$ our solution (38)–(41) takes the form

$$e^{-U}\equiv t^2=1-p^2-q^2, \tag{47}$$

$$e^{-M}=\frac{1}{trw}\left[t^2+2p^2q^2-2pqrw\cos(\alpha-\beta)\right], \tag{48}$$

$$\sinh W=\frac{2(pw\cos\alpha+qr\cos\beta)}{t^2+2p^2q^2-2pqrw\cos(\alpha-\beta)}, \tag{49}$$

$$e^{2V}=\frac{1+p^2w^2+q^2r^2+2pqrw\cos(\alpha-\beta)+2(pw\sin\alpha+qr\sin\beta)}{1+p^2w^2+q^2r^2+2pqrw\cos(\alpha-\beta)-2(pw\sin\alpha+qr\sin\beta)}, \tag{50}$$

$$p=u\theta(u),\quad q=v\theta(v),$$

which is the solution reported in Ref. 5. In the limit $\alpha=\beta=\pi/2$ this solution reduces to the solution by Khan and Penrose,

$$e^{-U}\equiv t^2=1-p^2-q^2, \tag{51}$$

$$e^{-M}=t^3\frac{r^{-1}w^{-1}}{(pq+rw)^2}, \tag{52}$$

$$W=0, \tag{53}$$

$$e^{V}=\frac{r+q}{r-q}\frac{w+p}{w-p}. \tag{54}$$

Finally, in the limit $\kappa\alpha=\beta\kappa=\pi/2$ for $n=2$, $\kappa=(3/2)^{1/2}$ the solution (38)–(41) reduces to

$$e^{-U}\equiv t^2=1-p^2-q^2, \tag{55}$$

$$e^{-M}=t^5\frac{(rw)^{-3/2}}{(pq+rw)^3}, \tag{56}$$

$$W=0, \tag{57}$$

$$e^{V}=\left[\left(\frac{w+p}{w-p}\right)\left(\frac{r+q}{r-q}\right)\right]^{(3/2)^{1/2}}, \tag{58}$$

which corresponds to the solution given by Szekeres. We have therefore generalized Szekeres' family to the case of linear but noncollinearly polarized plane gravitational waves for the case when Szekeres' parameters n_1 and n_2 are equal. In another publication we shall show that gravitational wave and stationary axially symmetric fields can be treated in a unified manner,[14] where the solution of one class enables us to derive solutions to the other class and vice-versa. This procedure can be extended to Einstein–Maxwell fields as well.

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APPENDIX: SINGULARITIES

In order to see the physical singularities of our solutions, we calculate the curvature invariants which are as follows:

$$\mathrm{Re}\psi_2=n^2\frac{u^{n-1}v^{n-1}}{rw}\theta(u)\theta(v)\left(\frac{-pqrw}{t^4}+\kappa^2\frac{(t^2+2p^2q^2)\cos(\alpha-\beta)-2pqrw}{(1-|\eta|^2)^2}\right),$$

$$\mathrm{Im}\psi_2=-\frac{\kappa^2n^2u^{n-1}v^{n-1}\theta(u)\theta(v)}{rw|\eta|^3(1-|\eta|^2)}\left(|\eta|^2-8p^2q^2r^2w^2\right)\cosh\omega\sin(\alpha-\beta),$$

$$\mathrm{Re}\psi_4=\frac{-\kappa n}{2r|\eta|(1+\cos^2\nu\sinh^2\omega)^{1/2}}\Bigg[\Bigg([(n-1)u^{n-2}\theta(u)+u^{n-1}\delta(u)]\Bigg(\frac{qw}{|\eta|}\cos\nu\sinh\omega\cdot\cosh\omega\cdot\sin(\alpha-\beta)+\frac{2\sin\nu Z}{1-|\eta|^2}\Bigg)$$

$$+nu^{2(n-1)}\theta(u)\Bigg\{\frac{qw}{|\eta|}\cos\nu\cdot\sinh\omega\cdot\cosh\omega\cdot\sin(\alpha-\beta)\Bigg(\frac{p(1-\kappa^2)}{r^2}-\frac{3p}{t^2}+\frac{(\kappa^2+1)|\eta|^2-1}{|\eta|^2(1-|\eta|^2)}+\frac{4\cosh\omega Z}{\sinh\omega r|\eta|(1-|\eta|^2)}\Bigg)$$

$$+\frac{2\sin\nu}{1-|\eta|^2}\Bigg[r(1-2q^2)-\frac{pqw}{r^2}(1+2r^2)\cos(\alpha-\beta)-\frac{1}{r}Z^2\Bigg(\frac{-3p}{t^2}-\frac{\kappa^2 p}{r^2}+\frac{(2\kappa^2-3)n^2+1}{|\eta|^2(1-|\eta|^2)}\Bigg)\Bigg]$$

$$-\kappa q^2w^2\frac{\sin\nu\sinh\omega\cdot\cosh\omega}{1+\cos^2\nu\sinh^2\omega}\cdot\frac{\sin^2(\alpha-\beta)}{r|\eta|^3}\Bigg\}\Bigg)\Bigg],$$

$$\mathrm{Im}\psi_4=-\frac{\kappa n}{2r|\eta|(1+\cos^2\nu\sinh^2\omega)}\Bigg[\Bigg([(n-1)u^{n-2}\theta(u)+u^{n-1}\delta(u)]\Bigg(\frac{2\cos\nu\cosh\omega}{1-|\eta|^2}Z$$

$$-\frac{qw\sin\nu\sinh\omega\sin(\alpha-\beta)}{|\eta|}\Bigg)+nu^{2(n-1)}\theta(u)\Bigg\{\frac{2\cos\nu\cdot\cosh\omega}{1-|\eta|^2}\Bigg[r(1-2q^2)-\frac{pqw}{r^2}$$

$$\times(1+2r^2)\cos(\alpha-\beta)+\frac{2(\kappa^2+2)|\eta|^2-3|\eta|^4-1}{r|\eta|^2(1-|\eta|^2)^2}Z^2-\frac{p}{1-|\eta|^2}\Bigg(\frac{3}{t^2}+\frac{\kappa^2}{r^2}\Bigg)\Bigg]$$

$$-\frac{qw}{|\eta|}\sin\nu\sinh\omega\sin(\alpha-\beta)\Bigg[p\Bigg(\frac{1-\kappa^2}{r^2}-\frac{3}{t^2}\Bigg)+\frac{2[(\kappa^2+1)|\eta|^2-1]}{r|\eta|^2(1-|\eta|^2)}Z\Bigg]$$

$$-\frac{\kappa q^2w^2}{r|\eta|^3}\cos\nu\sinh\omega\cdot\cosh^2\omega\sin^2(\alpha-\beta)-\frac{4\kappa qw}{r|\eta|^2}\sin\nu\cdot\cosh\omega\sin(\alpha-\beta)Z\Bigg\}\Bigg)\Bigg],$$

$$\psi_1=\psi_3=0,\quad \psi_0=\psi_4\quad (u\longleftrightarrow v,\alpha\longleftrightarrow\beta),$$

where

$$Z=pr(1-2q^2)+qw(1-2p^2)\cos(\alpha-\beta)\quad\text{and}\quad\cos\nu=\frac{\eta^\kappa+\bar\eta^\kappa}{2|\eta|^\kappa},\quad 2\cosh\omega=\Bigg(\frac{1+|\eta|}{1-|\eta|}\Bigg)^\kappa-\Bigg(\frac{1-|\eta|}{1+|\eta|}\Bigg)^\kappa$$

are to be substituted into these expressions. We observe that $r=w=0$ are singular surfaces expected from the focusing properties of the incoming waves. Same singularities arise from the roots of $|\eta|=0$. This is equivalent to $p^2+q^2-2p^2q^2=2pqrw\cos(\alpha-\beta)$, other roots of which depend on $(\alpha-\beta)$. The spacelike singularity $t^2=1-u^{2n}-v^{2n}=0$ reappears in the above invariants as well. We notice further that another singularity is provided by $1-|\eta|^2=0$, which is equivalent to $t^2=2pq[rw\cos(\alpha-\beta)-pq]$, which gives additional singularities depending on the values of α and β. For example, the choice $\alpha-\beta=(2n-1)\pi/2$ gives $t^2=-2p^2q^2$ which is satisfied for two symmetric hyperbolic branches starting at $(u=1, v=0)$ and $(v=1, u=0)$ and going in the increasing u,v directions so that it lies beyond the main singularity $t^2=0$. The singularity $t^2=0$ seems to be the essential feature of colliding plane gravitational waves.

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Convergence of the Debye expansion for the S matrix [a)]

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The convergence of the Debye expansion for the scattering of a scalar wave by a homogeneous sphere of complex refraction index, or, equivalently, of two particles interacting via a complex rectangular well (or barrier) potential, is considered. The interest of the results lies mainly in their applicability to hadron–nucleus and nucleus–nucleus collisions.

1. INTRODUCTION

Almost ten years ago, Nussenzveig showed the usefulness of the Debye expansion of the scattering matrix in the explanation of the atmospheric phenomena known as "rainbow' and "glory."[1] He considered a scalar wave of wave number k, incident on a transparent sphere of radius a and refraction index N. Using adimensional wave numbers,

$$\alpha=ka, \quad \beta=Nka, \tag{1.1}$$

for the exterior and interior regions of the spherical surface, the component of angular momentum l of the S matrix can be written as

$$S_l(k)=\frac{\alpha h_l^{(2)'}(\alpha)j_l(\beta)-\beta h_l^{(2)}(\alpha)j_l'(\beta)}{\alpha h_l^{(1)'}(\alpha)j_l(\beta)-\beta h_l^{(1)}(\alpha)j_l'(\beta)}, \tag{1.2}$$

where j_l, $h_l^{(1)}$, and $h_l^{(2)}$ are the familiar spherical Bessel and Hankel functions and the primes stand for derivatives with respect to their arguments. By denoting, as usual,

$$\lambda=l+\tfrac{1}{2} \tag{1.3}$$

and with the notation introduced by Nussenzveig,[1]

$$[z]=J_\lambda'(z)/J_\lambda(z), \tag{1.4a}$$

$$[1z]=H_\lambda^{(1)'}(z)/H_\lambda^{(1)}(z), \tag{1.4b}$$

$$[2z]=H_\lambda^{(2)'}(z)/H_\lambda^{(2)}(z), \tag{1.4c}$$

for the logarithmic derivatives of the cylindrical Bessel and Hankel functions, Eq. (1.2) can be put in the form

$$S_l(k)=-\frac{H_\lambda^{(2)}(\alpha)}{H_\lambda^{(1)}(\alpha)}\frac{[2\alpha]-N[\beta]}{[1\alpha]-N[\beta]}. \tag{1.5}$$

The Debye expansion of the S matrix arises when reflection and transmission coefficients on the interior (index 1) and exterior (index 2) sides of the spherical surface of radius a are defined according to

$$R_{11}=-\frac{[1\alpha]-N[1\beta]}{[1\alpha]-N[2\beta]}, \quad R_{22}=-\frac{[2\alpha]-N[2\beta]}{[1\alpha]-N[2\beta]}, \tag{1.6}$$

$$T_{12}=1+R_{11}, \quad T_{21}=1+R_{22}, \tag{1.7}$$

and used in Eq. (1.5). We obtain

$$S_l(k)=[H_\lambda^{(2)}(\alpha)/H_\lambda^{(1)}(\alpha)]\times\{R_{22}+T_{21}[H_\lambda^{(1)}(\beta)/H_\lambda^{(2)}(\beta)]\times(1-\rho)^{-1}T_{12}\}, \tag{1.8}$$

where

$$\rho=R_{11}H_\lambda^{(1)}(\beta)/H_\lambda^{(2)}(\beta). \tag{1.9}$$

Expanding $(1-\rho)^{-1}$ in a geometrical series, we arrive finally to the Debye expansion of the S matrix

$$S_l(k)=[H_\lambda^{(2)}(\alpha)/H_\lambda^{(1)}(\alpha)]\times\left\{R_{22}+T_{21}[H_\lambda^{(1)}(\beta)/H_\lambda^{(2)}(\beta)]\sum_{p=1}^{\infty}\rho^{p-1}T_{12}\right\}. \tag{1.10}$$

Each term of this expansion has a very clear physical interpretation in terms of multiple reflections of the wave in the interior of the sphere.[1]

The precedent formulation can be applied equally well to the nonrelativistic quantum mechanical scattering of a particle by a potential or of two particles interacting via a rectangular potential well or barrier,

$$V(r)=V_0\theta(a-r), \tag{1.11}$$

if one identifies the refraction index with

$$N=(1-2mV_0/\hbar^2k^2)^{1/2}, \tag{1.12}$$

m being the mass of the particle or the reduced mass of the system of two particles.

The Debye expansion method has been extended by Khare and Nussenzveig[2] to electromagnetic scattering. As suggested by Nussenzveig,[1] the Debye expansion can also be applied to problems of interest in nuclear physics, such as scattering of hadrons by nuclei or scattering between heavy ions. This has been done recently by Anni, Renna, and Taffara.[3] Also, in a different context, the Debye expansion has been used to explain the occurrence of resonances in a velocity-dependent potential.[4]

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The usefulness of Eq. (1.10) lies in the possibility of approximating the S matrix by the first terms of its expansion, that is, in the convergence of the Debye expansion. Such convergence has been proven by Nussenveig[1] in the case of a real refraction index (a real potential in the nuclear case) and conjectured by Anni, Renna, and Taffara[3] in the case of a complex refraction index (a complex potential in the corresponding nuclear case). Since the optical potentials in nuclear physics are necessarily complex, it has seemed to us worthwhile to analyze the convergence of the Debye expansion in the case of N complex. This is the purpose of this paper. In what follows we investigate, for different energies of the incident wave, the regions of the complex N plane for which

$$|\rho|<1 \tag{1.13}$$

and, therefore, the Debye expansion is convergent. We start with consideration, in Sec, 2, of particular regions of the N plane, namely the real and imaginary axes and the region far from the origin. Section 3 is devoted to the analysis of Eq. (1.13) in the case of very small and very high energies. In Sec. 4, numerical results corresponding to intermediate energies are reported. Finally, in Sec, 5, a discussion of the results is carried out.

It is interesting to notice that, in view of the relations (see Ref. 5, Eq. 9.1.39)

$$H_\lambda^{(1)}(z\exp\{\pi i\})=-\exp\{-\lambda\pi i\}H_\lambda^{(2)}(z), \tag{1.14a}$$

$$H_\lambda^{(2)}(z\exp\{-\pi i\})=-\exp\{\lambda\pi i\}H_\lambda^{(1)}(z), \tag{1.14b}$$

one can write

$$-z[1(-z)]=z[2z],\quad -z[2(-z)]=z[1z], \tag{1.15}$$

and hence, for λ half-integer (l physical),

$$\rho(l,k;-N)=1/\rho(l,k;N). \tag{1.16}$$

This reflection property tells us that if Eq. (1.13) holds at a given point, N, of the N plane, for the same angular momentum and energy we have $|\rho|>1$ at the symmetrical point, $-N$, with respect to the origin. So, it suffices in our discussion to consider only the right half of the N plane.

In the subsequent analysis, besides Eq. (1.15), the relations

$$\overline{z[1z]}=\bar{z}[2\bar{z}],\quad \overline{z[2z]}=\bar{z}[1\bar{z}],\quad \lambda \text{ real}, \tag{1.17}$$

obtained from (see Ref. 5, Eq. 9.1.40)

$$\overline{H_\lambda^{(1)}(z)}=H_\lambda^{(2)}(\bar{z}),\quad \overline{H_\lambda^{(2)}(z)}=H_\lambda^{(1)}(\bar{z}),\quad \lambda \text{ real}, \tag{1.18}$$

will prove to be useful.

2. SPECIAL VALUES OF THE REFRACTION INDEX

The convergence of the Debye expansion in the case of real N has already been considered by Nussenzveig. In fact, he has proven[1] that Eq. (1.13) holds at all energies not only for physical values of the angular momentum, but for any real value of λ. In this section we shall discuss the two cases of pure imaginary N and of $|N|\gg 1$.

A. Positive pure imaginary refraction index

For a pure imaginary refraction index, the Hankel function $H_\lambda^{(2)}(\beta)$ corresponding to odd angular momentum ($\lambda=$ odd $+\frac{1}{2}$) vanishes at a certain energy,[6] making singular the quotient $H_\lambda^{(1)}(\beta)/H_\lambda^{(2)}(\beta)$and the denominator of R_{11}. The form Eq. (1.9) is not suited for this case, as it would appear undetermined at such energy. Instead, we prefer to use the equivalent expression.

$$\rho^{-1}=1-2J_\lambda(\beta)/H_\lambda^{(1)}(\beta)$$

$$-\frac{4i}{\pi[H_\lambda^{(1)}(\beta)]^2\{\alpha[1\alpha]-\beta[1\beta]\}}, \tag{2.1}$$

obtained from Eq. (1.9) by replacing (see Ref. 5, Eq. 9.1.4)

$$H_\lambda^{(2)}(z)=2J_\lambda(z)-H_\lambda^{(1)}(z) \tag{2.2}$$

and recalling the value of the Wronskian of the two Hankel functions (see Ref. 5, Eq. 9.1.17),

$$W\{H_\lambda^{(1)}(z),H_\lambda^{(2)}(z)\}=-4i/\pi z. \tag{2.3}$$

Let us start with the particular case of very low energies, that is,

$$\alpha\to 0,\quad |\beta|\to 0. \tag{2.4}$$

We assume $\lambda>1$, the case $\lambda=\frac{1}{2}$ being considered in Sec. 4. From the ascending series expansions of the Bessel and Hankel functions (see Ref. 5, Eq. 9.1.10) it is easy to obtain, retaining only dominant terms,

$$J_\lambda(z)\simeq(z/2)^\lambda/\Gamma(\lambda+1),\quad |z|\to 0 \tag{2.5}$$

$$H_\lambda^{(1)}(z)\simeq -H_\lambda^{(2)}(z)$$

$$\simeq(-i/\pi)\Gamma(\lambda)(z/2)^{-\lambda},\quad |z|\to 0. \tag{2.6}$$

Replacing Eqs. (2.5) and (2.6) in Eq. (2.1), it becomes

$$\rho^{-1}\simeq 1-2\pi i(\beta/2)^{2\lambda}[\Gamma(\lambda)]^{-2}$$

$$\times(1/\lambda-2/\{\alpha[1\alpha]-\beta[1\beta]\}). \tag{2.7}$$

The convergence of the Debye expansion, Eq. (1.13), requires

$$i(\beta/2)^{2\lambda}\mathrm{Re}(1/\lambda-2/\{\alpha[1\alpha]-\beta[1\beta]\})<0. \tag{2.8}$$

Being $\lambda=l+\frac{1}{2}$ ($l=1,2,3,\cdots$), we can use (see Ref. 5, Eqs. 10.1.1, 10.1.16 and 10.1.17)

$$H_\lambda^{(1)}(z)=(2/\pi)^{1/2}i^{-l-1}z^{-1/2}\exp\{iz\}$$

$$\times\sum_{n=0}^{l}(\lambda,n)(-2iz)^{-n}, \tag{2.9}$$

$$H_\lambda^{(2)}(z)=(2/\pi)^{1/2}i^{l+1}z^{-1/2}\exp\{-iz\}$$

$$\times\sum_{n=0}^{l}(\lambda,n)(2iz)^{-n}, \tag{2.10}$$

with

$$(\lambda,n)=(l+n)!/n!(l-n)!, \tag{2.11}$$

to obtain the exact expressions

$$z[1z]=-\tfrac{1}{2}+iz$$

$$+\sum_{n=0}^{l}(-n)(\lambda,n)\ (-2iz)^{-n}$$

$$\times\left(\sum_{n=0}^{l}(\lambda,n)(-2iz)^{-n}\right)^{-1}, \tag{2.12}$$

$$z[2z]=-\tfrac{1}{2}-iz$$

$$+\sum_{n=0}^{l}(-n)(\lambda,n)(2iz)^{-n}$$

$$\times\left(\sum_{n=0}^{l}(\lambda,n)(2iz)^{-n}\right)^{-1}. \tag{2.13}$$

In the case under consideration, we can approximate

$$\mathrm{Re}\{\alpha[1\alpha]-\beta[1\beta]\}\simeq\alpha^2(1+|N|^2)/(2l-1),\quad \alpha\to 0, \tag{2.14a}$$

$$\mathrm{Im}\{\alpha[1\alpha]-\beta[1\beta]\}=\mathrm{Im}\{\alpha[1\alpha]\}$$

$$\simeq\alpha^{2l+1}/[(2l-1)!!]^2,\quad \alpha\to 0. \tag{2.14b}$$

Equation (2.14a) shows that the last factor in the left-hand side of Eq. (2.8) is negative independently of the value of N. The condition Eq. (2.8) becomes equivalent to

$$i^{2l+2}>0, \tag{2.15}$$

which is satisfied for odd values of l. So, we can conclude that in the case of positive pure imaginary refraction index, at low energies, the Debye expansion for an odd l-wave converges, no matter which value $\mathrm{Im}N$ takes. For even l-waves we find $|\rho|>1$ and the expansion becomes nonconvergent.

Now, let us examine the possibility of having $|\rho|=1$ for $|N|\to 0$ at intermediate values of the energy. Since $|\beta|\to 0$, Eq. (2.7) remains still valid. The condition $|\rho|=1$ becomes approximately equivalent to

$$\mathrm{Re}(1/\lambda-2/\{\alpha[1\alpha]-\beta[1\beta]\})=0. \tag{2.16}$$

From Eq. (2.12), it is evident that, to the order of approximation retained, we can replace $\beta[1\beta]$ in Eq. (2.16) by its approximate value, $-\lambda$. Then Eq. (2.16) reduces to

$$|\alpha[1\alpha]|=\lambda. \tag{2.17}$$

By replacing the real and imaginary parts of $\alpha[1\alpha]$ by their exact expressions,[4] Eq. (2.17) can be put in the form

$$s=\sum_{n=0}^{l}(2l+1-n)\,\frac{(2l-n)!(2l-2n)!}{n![(l-n)!]^2}(4s)^{n-l}$$

$$\times\sum_{n=0}^{l}n\,\frac{(2l-n)!(2l-2n)!}{n![(l-n)!]^2}(4s)^{n-l}, \tag{2.18}$$

where

$$s=\alpha^2 \tag{2.19}$$

represents an adimensional energy parameter. It is immediate to check that Eq. (2.18) has only one solution for positive s.

Finally, let us consider what happens when the energy reaches very high values. More precisely, let us study the case $\alpha\to\infty$, $|\beta|$ being finite. From Eqs. (2.12) and (2.13) we obtain the approximate expressions

$$z[1z]\sim iz-\tfrac{1}{2},\quad |z|\to\infty, \tag{2.20}$$

$$z[2z]\sim -iz-\tfrac{1}{2},\quad |z|\to\infty, \tag{2.21}$$

The first of these expressions, replaced for $\alpha[1\alpha]$ in

$$R_{11}=-\frac{\alpha[1\alpha]-\beta[1\beta]}{\alpha[1\alpha]-\beta[2\beta]}, \tag{2.22}$$

allows us to conclude that $R_{11}\to -1$ as the energy increases. If we are interested in the intersection of the line $|\rho|=1$ in the complex N plane with the positive imaginary axis, we ought to search for imaginary values of β satisfying

$$|H_\lambda^{(1)}(\beta)/H_\lambda^{(2)}(\beta)|=1, \tag{2.23}$$

which can be written, using Eqs. (2.9) and (2.10), in the form

$$\exp\{-2y\}=\sum_{n=0}^{l}(\lambda,n)(-2y)^n$$

$$\times\left(\sum_{n=0}^{l}(\lambda,n)(2y)^n\right)^{-1}, \tag{2.24}$$

or, equivalently,

$$\exp\{-2y\}=\sum_{n=0}^{l}(\lambda,l-n)(-2y)^n$$

$$\times\left(\sum_{n=0}^{l}(\lambda,l-n)(2y)^n\right)^{-1}, \tag{2.25}$$

where we have denoted

$$\beta=iy, \tag{2.26}$$

y being positive. It is easy to see that Eq. (2.25) has only one solution for odd l and no solution for even l.

The present results allow us to draw conclusions about the convergence of the Debye expansion for positive pure imaginary refraction index, as the energy varies from zero to infinity. For $l=1,3,5,\ldots$, the expansion is convergent at zero energy for all values of $\mathrm{Im}N$. This result remains valid, as the energy increases, until the value given by the solutio nof Eq. (2.18) is reached. Then, the expansion is convergent for $\mathrm{Im}N$ above a point which, starting from the origin at the energy quoted, goes up as the energy increases, stops and reverses its motion, approaching asymptotically the origin as the energy

becomes infinite, in such a manner that $\alpha \mathrm{Im}N$ tends to the constant given by the solution of Eq. (2.25). For $l=2,4,6,...$, the expansion is nonconvergent at zero energy for any ImN. As the energy increases, the expansion becomes convergent for ImN above a point that, coming from infinity, goes towards the origin and reaches it for an energy given by the solution of Eq. (2.18). For higher energies, the expansion is convergent for all values of ImN.

B. Very high complex refraction index

In the case $|N|\to\infty$ it turns out $|\beta|\to\infty$ and we can use Eqs. (2.20) and (2.21), for $\beta[1\beta]$ and $\beta[2\beta]$ in Eq. (2.22), to obtain

$$R_{11}\sim\frac{\alpha[1\alpha]-i\beta+\frac{1}{2}}{\alpha[1\alpha]+i\beta+\frac{1}{2}}, \quad |\beta|\to\infty. \tag{2.27}$$

It is clear that

$$R_{11}\sim 1 \quad \text{for} \quad |N|\to\infty. \tag{2.28}$$

The convergence of the Debye expansion is in this case determined mainly by the quotient of the two Hankel functions, which can be approximate in the form

$$|H_\lambda^{(1)}/H_\lambda^{(2)}|\sim\exp\{-2\alpha\mathrm{Im}N\}, \quad |\beta|\to\infty. \tag{2.29}$$

In view of Eqs. (2.28) and (2.29), we can conclude that the line

$$|\rho|=1, \tag{2.30}$$

delimiting the convergence region, tends asymptotically to the real axis as $\mathrm{Re}N\to+\infty$. It is not difficult to see that the line $|\rho|=1$ is tangent to the real axis from below. It is evident from Eq. (2.29) that, far from the real axis, the Debye expansion is convergent in the first quadrant and nonconvergent in the fourth one. The separation line between the convergence and nonconvergence regions must lie, for $\mathrm{Re}N\to+\infty$, below the real axis, since the entire real positive axis belongs to the convergence region.

In conclusion, for points N far from the origin, the Debye expansion is convergent in the first quadrant. The rapidity of the convergence can be inferred from Eqs. (2.28) and (2.29).

3. EXTREME VALUES OF THE ENERGY

In this section we consider the convergence of the Debye expasion for any complex N in the two limiting cases of very low and very high energies.

A. Case of very low energy

Let us suppose that $\alpha\to 0$ and, hence, $|\beta|\to 0$. We can use approximate expressions for the Bessel and Hankel functions appearing in the definition of ρ, Eq. (1.9). It is convenient, however, to put ρ in the form

$$\rho=1-\frac{2J_\lambda(\beta)}{H_\lambda^{(2)}(\beta)} + \frac{4i}{\pi[H_\lambda^{(2)}(\beta)]^2\{\alpha[1\alpha]-\beta[2\beta]\}}, \tag{3.1}$$

obtained from Eq. (1.9) similary to Eq. (2.1). Let us assume $\lambda>1$, the case $\lambda=\frac{1}{2}$ being considered in Sec. 4. Replacing Eqs. (2.5) and (2.6) in Eq. (3.1), it becomes

$$\rho\simeq 1+2\pi i[\Gamma(\lambda)]^{-2}(\beta/2)^{2\lambda}(1/\lambda-2/\{\alpha[1\alpha]-\beta[2\beta]\}). \tag{3.2}$$

Bearing in mind Eqs. (2.12) and (2.13), we can approximate further Eq. (3.2) to obtain

$$\rho\simeq 1+2\pi i(\lambda-1)[\Gamma(\lambda)]^{-2}(\alpha/2)^{2\lambda-2}N^{2\lambda}/(1-N^2). \tag{3.3}$$

It is evident from Eq. (3.3) that the convergence at low energies is very slow ($|\rho|\simeq 1$) and requires

$$\mathrm{Re}[-iN^{2\lambda}/(1-N^2)]<0, \tag{3.4}$$

which implies

$$\mathrm{Im}[N^{2\lambda}/(1-N^2)]<0, \tag{3.5}$$

or, equivalently,

$$\mathrm{Im}(N^{2\lambda}-|N^2|^2N^{2\lambda-2})<0. \tag{3.6}$$

Denoting

$$M=|N|, \quad \Theta=\arg N, \tag{3.7}$$

the condition Eq. (3.6) can be written in the form

$$F(M,\Theta)\equiv\sin(2\lambda\Theta)-M^2\sin[(2\lambda-2)\Theta]<0. \tag{3.8}$$

In the analysis of Eq. (3.8) it is convenient to consider in the first quadrant of the N plane $2l$ regions A_q, $q=1,2,...,2l$, defined in the form

$$A_{2p-1}: \ (p-1)\pi/(2\lambda-2)<\Theta<p\pi/2\lambda, \quad p=1,2,...,l, \tag{3.9a}$$

$$A_{2p}: \ p\pi/2\lambda<\Theta<p\pi/(2\lambda-2), \quad p=1,2,...,l, \tag{3.9b}$$

It is then obvious to check the following results:

(i) region A_{2p-1}:

(a) p odd; $F(M,\Theta)<0$

$$\text{for } M^2>\sin(2\lambda\Theta)/\sin[(2\lambda-2)\Theta], \tag{3.10a}$$

(b) p even; $F(M,\Theta)<0$

$$\text{for } M^2<\sin(2\lambda\Theta)/\sin[(2\lambda-2)\Theta], \tag{3.10b}$$

(ii) region A_{2p}:

(a) p odd; $F(M,\Theta)<0$ for all M, (3.11a)

(b) p even; $F(M,\Theta)>0$ for all M. (3.11b)

As far as $F(M,\Theta)$ is an odd function of Θ, it is evident that F presents in the fourth quadrant the opposite sign of that in the complex conjugate quadrant. For a better visualization of the results, Eqs. (3.10) and (3.11), we have represented them in Fig. 1 for the particular case $l=4$.

Of course, our precedent analysis is valid only for points not far from the origin. Otherwise, the assumption $|\beta|\to 0$ should not be valid and we could not make use of Eqs. (2.5) and (2.6). Far from the origin, the analysis made in Sec. 2 B would stand.

B. Case of very high energy

Now, let us assume $\alpha\to\infty$. Of course, we have also $|\beta|\to\infty$, and the approximate expressions Eqs. (2.20), (2.21), and (2.29) can be used. We so obtain

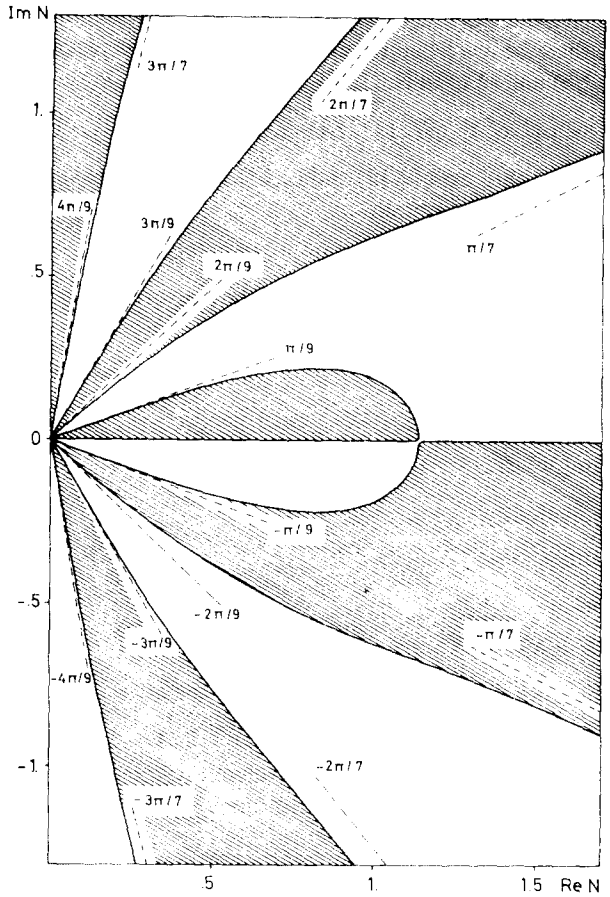

FIG. 1. Low energy limit of the convergence and nonconvergence regions of the Debye expansion for scattering of a scalar wave, of angular momentum $l=4$, by a homogeneous sphere of complex refraction index N. The expansion is nonconvergent in the shadowed regions. The curves delimiting the convergence regions become tangent to the dashed straight lines. The real axis belongs to the convergence region.

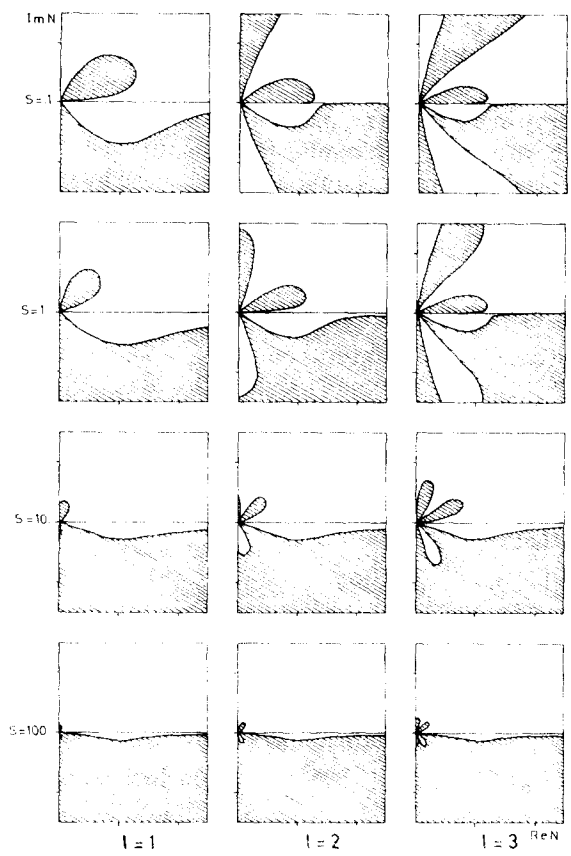

FIG. 2. Convergence and nonconvergence (shadowed) regions for waves of angular momenta $l=1,2,3$, and for different values of the energy parameter $s=0.1$, 1.0, 10.0, 100.0. The divisions of the real and imaginary axes correspond to the unit.

$$|\rho|\sim\exp(-2\alpha\,\mathrm{Im}N)|(1-N)/(1+N)|. \tag{3.12}$$

At high energy, the Debye expansion becomes convergent in all the first quadrant and, in the fourth quadrant, above a line which starts at the origin, goes right and downwards, presents a minimum at $\mathrm{Re}N\simeq 1$ and goes right and upwards, to be asymptotically tangent to the real axis from below.

4. INTERMEDIATE ENERGIES

At intermediate energies we cannot use aproximate expressions for the Bessel and Hankel functions, and a discussion of Eq. (1.13) becomes difficult. In the case $l=0$, however, such functions have a very simple form, which allows us to write

$$\rho=\exp(2i\beta)(1-N)/(1+N), \tag{4.1}$$

and, therefore,

$$|\rho|=\exp(-2\alpha\,\mathrm{Im}N)|(1-N)/(1+N)|. \tag{4.2}$$

The convergence region in the case $l=0$ shows the aspect we have just described above, at the end of the precedent section, in the case of very high energy.

For $l\neq 0$, we have done a numerical analysis of Eq. (1.13). Our results are reported in Fig. 2. We can see in there the evolution of the convergence region, as the energy increases, from the situation described in Sec. 3 A, to that of 3 B: The loops delimiting the convergence region reduce their size. The behavior on the imaginary axis described in Sec. 2 A, is now made clear by the counterclockwise rotation of the loops as the energy increases.

5. DISCUSSION

As pointed out in Sec. 1, one of the most interesting applications of the Debye expansion is in the study of nucleus-nucleus and hadron-nucleus collisions. Our analysis of the convergence of such expansion has been limited to a (complex) square well potential. In fact, the Debye expansion has not yet been generalized to potential shapes different from the square well, although some of the conclusions of our precedent analysis would remain valid in the case of more realistic potentials, such as Saxon–Woods potentials.

In the case of low energies (more precisely, in the case of low values of the external wave number times the range parameter), the convergence of the Debye expansion becomes very sensitive to the precise values of the parameters of the potential. Furthermore, since $|\rho|\simeq 1$ in all the N plane, the convergence would result very slow and many terms of the expansion should be retained in order to obtain an acceptable accuracy.

At intermediate energies, the Debye expansion becomes rapidly convergent for strongly absorptive ($\mathrm{Im}N > 0$) potentials and divergent for strongly emissive ($\mathrm{Im}N < 0$) potentials, as it should be expected. For weakly absorptive or emissive potentials, the convergence depends on the particular values of the parameters involved.

At high energies, the expansion is convergent for absorptive potentials and divergent for emissive potentials. The rapidity of the convergence can be conjectured from the approximate relation

$$|\rho| \sim \exp(-2\alpha \mathrm{Im}\langle N\rangle). \tag{5.1}$$

where α represents the product of the external wave number times the range parameter of the potential and $\langle N\rangle$ stands for an average value of the refraction index.

The extension of our study of the convergence of the Debye expansion to potentials with a Coulomb tail would present, in principle, no difficulty. It would suffice to replace the Whittaker functions for the Hankel functions in the Coulombian region.

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Relativistic scattering of model particles

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Relativistic scattering of particles belonging to an irreducible representation (irrep) of the 11-parameter Weyl Lie algebra w is studied. The irrep of w is realized on a manifold $R^3 \times T$ where $T = [0,\pi]$. From the corresponding wavefunctions a local relativistic field is constructed which is coupled to itself in such a way that w is respected. Scattering is studied in the Born approximation.

INTRODUCTION

If hadrons are composed of constituents then hadron–hadron interactions is a manybody problem for which we do not know the fundamental interaction. However, even knowledge of this fundamental interaction between the constituents might not be of much use in predicting the outcome of hadron scattering experiments at present, due to computational difficulties as in QCD. In view of this it might be useful to find other appoaches to the problem. We could, e.g., consider the fundamental interaction to create in the first place the bound states of the system, i.e., essentially determine the mass spectrum and then secondly study scattering of these bound states on each other. Along these lines one could then first try to solve the bound state problem, by using a mass spectrum generating relativistic Lie algebra $\mathfrak{g}$ (=containing the Poincaré Lie algebra) and look for a Poincaré partially integrable irreducible representation of $\mathfrak{g}$ with nontrivial mass content. Over the carrier space of such an irreducible representation (irrep) we could then construct a Fock space and an associated free field. This field should then be coupled to itself in such a way that the interaction respects the Lie algebra $\mathfrak{g}$ so that $\mathfrak{g}$ can be realized as a charge algebra in terms of the interacting field. It could then be hoped that already low order perturbation theory would give relatively detailed information about cross sections, particle widths, resonances, etc.

This paper is devoted to a realization of this program for a simple model, hence the particles are called model particles. We will study scattering of particles belonging to an irreducible representation of the 11-parameter Weyl Lie algebra $\mathfrak{w}$. Here $\mathfrak{w}$ acts as a spectrum-generating Poincaré integrable Lie algebra[1,2] and an irreducible representation of $\mathfrak{w}$ corresponds quantum mechanically to an elementary object. The subspaces in the decomposition of such an irrep of $\mathfrak{w}$ into irreps of the Poincaré group corresponds to different types of elementary particles. The irreps of $\mathfrak{w}$ are realized on a Hilbert space E of functions over a four-dimensional manifold $R^3 \times T$, where $T=[0,\pi]$. T represents the manifold for the inner structure of the particle and to each vibrational mode of the object with "length" π there corresponds a particle with mass $m_0 k$ (where $k=1,2,3\cdots$). This representation can be mapped into a Hilbert space $\mathscr{H}(x^0)$ endowed with a time parameter x^0. The functions in $\mathscr{H}(x^0)$ are the positive energy solutions to the wave equation $(\Box - m_0^2\partial_q^2)\varphi(x,q)=0$ ($x\in R^4$, $q\in T$). In the Fock space $\Gamma(\mathscr{H}(x^0))$ over $\mathscr{H}(x^0)$ we can define fields $\Phi(x,q)$ fulfilling a field equation of the same form as the wave equation in $\mathscr{H}(x^0)$. This field equation and the Fock space representation of $\mathfrak{w}$ can be derived from a Lagrangian $\mathscr{L}_0$ by applying a variational principle on the corresponding action.

We then introduce interaction by adding an extra term to the action integral. This term can be chosen in such a way that the (local) Weyl algebra symmetry is preserved. Starting from the action, we can set up expressions for the eleven generators of the Weyl algebra satisfying the appropriate commutation relations. In this model scale invariance is broken intrinsically since the dilatation generator is not integrable to an operator for finite dilatations.

Finally we set up the perturbation expansion for the S matrix and give the corresponding Feynman rules. As an example we apply this technique on the problem of two-body scattering and calculate the S-matrix element in lowest order Born approximation and then we determine explicitly the high energy behavior for two different interaction terms.

THE "BOUND-STATE PROBLEM"

The Weyl Lie algebra $\mathfrak{w}$ has the structure

$$\mathfrak{w} = (\mathfrak{t}^4 \oplus \mathfrak{so}(3,1)) \in R_+. \tag{2.1}$$

$\mathfrak{w}$ is spanned by the Poincaré generators P^μ and $M^{\mu\nu}$ and the dilatation generator D. Besides the ordinary commutation relations between P^μ and $M^{\mu\nu}$ these generators satisfy

$$[D,P^\mu] = -iP^\mu, \tag{2.2a}$$

$$[D,M^{\mu\nu}] = 0. \tag{2.2b}$$

Let E be the Hilbert space $L^2(R^3,d^3x) \otimes L^2(T,dq)$, where $T=[0,\pi]$, and let a function $g(\bar{x},q)\in E$ have the Fourier resolution

$$g(\bar{x},q) = \sum_{k=1}^{\infty} \int_{R^3} d^3p\,(2\pi)^{-3/2}(\pi/2)^{-1/2}\, e^{i\bar{p}\bar{x}}\, \sin kq\, \tilde{g}_k(\bar{p}). \tag{2.3}$$

The operator $V = -\Delta - m_0^2\partial_q^2$ is positive on the subspace $\mathscr{S}(R^3) \otimes C(T)_0^2$ in E, where we let $C(T)^k_{1,m,\ldots}$ denote a set of k times continuously differentiable functions on T such that their lth, mth, etc., derivatives vanish at $q=0$ and $q=\pi$. Then for $g(\bar{x},q)\in\mathscr{S}(R^3) \otimes C(T)_0^2$ we can define a positive operator $V^{1/2}$ via spectrality, i.e.,

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$$(V^{1/2}g)(\bar{x},q)=\sum_k \int d^3p\,(2\pi)^{-3/2}e^{i\bar{p}\bar{x}}\sin kq$$

$$\times(\bar{p}^2+m_0^2k^2)^{1/2}\tilde{g}_k(\bar{p}). \tag{2.4}$$

Similarly we can define the operator $V^{-1/2}$ on all of E since it is bounded.

Letting $g(\bar{x},q)\in S=\mathscr{S}(R^3)\otimes C(T)^{\infty}_{0,1,2,4,6,\cdots}$, we can set up a representation of $\mathfrak{w}$ as follows:

$$P^0g(\bar{x},q)=V^{1/2}g(\bar{x},q), \tag{2.5a}$$

$$\bar{P}g(\bar{x},q)=-i\bar{\nabla}g(\bar{x},q), \tag{2.5b}$$

$$\bar{J}g(\bar{x},q)=-i\bar{x}\times\bar{\nabla}g(\bar{x},q), \tag{2.5c}$$

$$\bar{K}g(\bar{x},q)=(-V^{1/2}\bar{x}-\tfrac{1}{2}V^{-1/2}\bar{\nabla})g(\bar{x},q), \tag{2.5d}$$

$$Dg(\bar{x},q)=\tfrac{1}{2}i(\bar{x}\bar{\nabla}+\bar{\nabla}\bar{x}+q\partial_q+\partial_q q)g(\bar{x},q), \tag{2.5e}$$

where $J_i=-\frac{1}{2}\epsilon_{ikl}M^{kl}$ and $K_i=M_{0i}$.[3]

Theorem 1: (a) The operators P^μ, $M^{\mu\nu}$ and D defined above are symmetric on S.

(b) P^μ, $M^{\mu\nu}$, and D map S into subspaces on which they all are symmetric.

(c) The commutation relation of $\mathfrak{w}$ are fulfilled on S.

Proof: (a) P^0 and $\bar{K}$ are symmetric on $\mathscr{S}(R^3)\otimes C(T)^{\infty}_0$ since V is positive on that domain. $\bar{P}$ and $\bar{J}$ are symmetric on $\mathscr{S}(R^3)\otimes L^2(T,dq)$ and D is symmetric on $\mathscr{S}(R^3)\otimes C(T)^1_0$. Hence we conclude that P^μ, $M^{\mu\nu}$, and D are symmetric on S.

(b) P^μ and $M^{\mu\nu}$ map $\mathscr{S}(R^3)\otimes C(T)^{\infty}_{0,2,4,\cdots}$ into itself and D maps $\mathscr{S}(R^3)\otimes C(T)^{\infty}_{0,1}$ into $\mathscr{S}(R^3)\otimes C(T)^{\infty}_0$. Hence P^μ, $M^{\mu\nu}$ and D map S into subspaces of E on which they all are symmetric.

(c) It is trivial to verify that the commutation relations of $\mathfrak{w}$ are fulfilled on S.

Definition 1: A representation of $\mathfrak{w}$ is "weakly" Schur irreducible if every bounded operator A that commutes strongly with P^μ and $M^{\mu\nu}$ and weakly with D is a multiple of the identity operator.

Theorem 2: The representation of $\mathfrak{w}$ defined in (2.5a)–(2.5e) is "weakly" Schur irreducible.

Proof: Consider a bounded operator A which commutes strongly with P^μ and $M^{\mu\nu}$. A is then a multiple of the identity on every eigenspace of the mass^2 operator $M^2=P_\mu P^\mu=-m_0^2\partial_q^2$. Hence $A=\Sigma_1^\infty a_kI_k$, where I_k projects on the eigenspace on which $M^2=m_0^2k^2$. Assume now that A commutes weakly with D, i.e.,

$$(f;(AD-DA)g)=0, \quad \text{for all } f,g\in S. \tag{2.6}$$

Inserting the Fourier expansions (2.4) of f and g and using the definition (2.5e) for D, we obtain

$$\sum_{k,l}(a_k-a_l)\int d^3p\,\tilde{f}_k^*(\bar{p})F_{kl}\tilde{g}_l(\bar{p})=0, \tag{2.7a}$$

where

$$F_{kl}=2/\pi\int_0^\pi \sin kq\,\tfrac{1}{2}i(q\partial_q+\partial_q q)\sin lq\,dq$$

$$=\begin{cases}\dfrac{(-1)^{k+l+1}2kl}{k^2-l^2}\neq 0, & \text{for } k\neq l\\ 0, & \text{for } k=l\end{cases} \tag{2.7b}$$

(2.7) implies that $a_k=a_l$ for all k and l and hence A is a multiple of the identity and the theorem is proved. Q.E.D.

We have thus found an irrep of $\mathfrak{w}$ in E with mass spectrum $m_0,2m_0,3m_0,\cdots$. This mas spectrum corresponds to the choice $g(\bar{x},0)=g(\bar{x},\pi)=0$ of the boundary conditions in this Sturm–Liouville problem. Other choices are possible, but this one corresponds to the "reflecting walls" of an infinite square-well potential which we prefer on physical grounds and also because of simplicity.

Next we shall set up an equivalent representation of $\mathfrak{w}$ in a Hilbert space $\mathscr{H}(x^0)$. With each vector $g(\bar{x},q)\in E$ we can associate a new vector

$$\varphi(x,q)=G(x^0)g(\bar{x},q)=2^{-1/2}V^{-1/4}e^{-ix^0V^{1/2}}g(\bar{x},q). \tag{2.8}$$

The operator $G(x^0)$ can be extended to all of E since it is bounded relative the norm in E. Then we define a new scalar product for the new vectors (2.8),

$$(\varphi_1;\varphi_2)_{x^0}=(g_1;g_2). \tag{2.9}$$

The set (2.8) of functions and the scalar product (2.9) defines a new Hilbert space $\mathscr{H}(x^0)$ and $G(x^0)$ is an isometric transformation from E to $\mathscr{H}(x^0)$. Now let $\varphi(x,q)\in S(x^0)=G(x^0)S$. We can then set up the following representation of $\mathfrak{w}$ on $S(x^0)$ in $\mathscr{H}(x^0)$ which is equivalent to the representation (2.5a)–(2.5e) of $\mathfrak{w}$ in E:

$$P^0\varphi(x,q)=G(x^0)V^{1/2}g(\bar{x},q)=V^{1/2}\varphi(x,q)=i\partial^0\varphi(x,q), \tag{2.10a}$$

$$\bar{P}\varphi(x,q)=G(x^0)(-i\bar{\nabla})g(\bar{x},q)=-i\bar{\nabla}\varphi(x,q), \tag{2.10b}$$

$$\bar{J}\varphi(x,q)=G(x^0)(-i\bar{x}\times\bar{\nabla})g(\bar{x},q)=-i\bar{x}\times\bar{\nabla}\varphi(x,q), \tag{2.10c}$$

$$\begin{aligned}\bar{K}\varphi(x,q)&=G(x_0)(V^{1/2}\bar{x}-\tfrac{1}{2}V^{-1/2}\bar{\nabla})g(\bar{x},q)\\&=(-\bar{x}V^{1/2}-ix^0\bar{\nabla})\varphi(x,q)\\&=-i(x^0\bar{\nabla}+\bar{x}\partial^0)\varphi(x,q),\end{aligned} \tag{2.10d}$$

$$\begin{aligned}D\varphi(x,q)&=G(x^0)\tfrac{1}{2}i(\bar{x}\bar{\nabla}+\bar{\nabla}\bar{x}+q\partial_q+\partial_q q)g(\bar{x},q)\\&=\tfrac{1}{2}i(-2ix^0V^{1/2}+\bar{x}\bar{\nabla}+\bar{\nabla}\bar{x}+q\partial_q+\partial_q q-1)\\&\quad\times\varphi(x,q)\\&=i(x^\mu\partial_\mu+q\partial_q+\tfrac{3}{2})\varphi(x,q).\end{aligned} \tag{2.10e}$$

Because of the third equality of (2.10a) we find that the functions $\varphi(x,q)\in\mathscr{H}(x^0)$ are the positive energy solutions to the generalized Klein–Gordon equation

$$(\Box-m_0^2\partial_q^2)\varphi(x,q)=0. \tag{2.11}$$

We also find that the scalar product (2.9) in $\mathscr{H}(x^0)$ can be expressed as a generalized Klein–Gordon scalar product since

$$(\varphi_1;\varphi_2)_{x^0}=(g_1;g_2)=\int g_1^*g_2\,d^3x\,dq$$

$$= \int (e^{-ix^0 V^{1/2}} g_1)^* e^{-ix^0 V^{1/2}} g_2 d^3x\, dq$$

$$= \int \varphi_1^* i \overleftrightarrow{\partial}_0 \varphi_2 d^3x\, dq. \tag{2.12}$$

The construction of the $\mathfrak{w}$-representation in E instead of the more natural one in $\mathscr{H}(x^0)$ has been done since it is only by direct or indirect reference to the representation in E that Theorems 1 and 2 can be proven.

3. FIELD THEORY

In Sec. 2 we set up (equivalent) representations of $\mathfrak{w}$ in E and $\mathscr{H}(x^0)$. In this section we shall construct the analog representation in the Fock space $\Gamma(E)$ over E. We then show that the representation in $\Gamma(E)$ is equivalent to a representation derived from a Lagrangian free-field theory.

We start by defining the symmetric Fock space $\Gamma(E)$ over E.[4-6]

$$\Gamma(E) = E^{(0)} \oplus E^{(1)} \oplus E^{(2)} \oplus \cdots, \tag{3.1a}$$

where

$$E^{(n)} = \sigma(E \otimes E \otimes E \otimes \cdots) = \sigma(E^{\otimes n}), \tag{3.1b}$$

and where σ is the symmetrizer. We let $\Gamma(E)$ have the natural scalar product induced by the scalar product in E.

Let $|\bar{p},k\rangle$ denote a one-particle state with momentum $\bar{p}$ and mass $m_0 k$ and with the following normalization

$$\langle \bar{p},k | \bar{p}',k' \rangle = \delta^3(\bar{p}-\bar{p}')\delta_{kk'}. \tag{3.2}$$

Let $a_k^+(\bar{p})$ be the creation operator of such a state and $a_k(\bar{p})$ the corresponding annihilation operator. Then

$$[a_k(\bar{p}), a_k^+(\bar{p})] = \delta^3(\bar{p}-\bar{p}')\delta_{kk'}. \tag{3.3}$$

Next let $|\bar{x},q\rangle$ denote the state of a particle localized at $(\bar{x},q)$ and let $\psi^+(\bar{x},q)$ and $\psi(\bar{x},q)$ be the corresponding creation and annihilation operators. We get

$$\psi(\bar{x},q) = \sum_k \int d^3p\, (2\pi)^{-3/2} (\pi/2)^{-1/2} e^{i\bar{p}\bar{x}} \sin kq\, a_k(\bar{p}) \tag{3.4a}$$

and

$$[\psi(\bar{x},q), \psi^+(\bar{x}',q')] = \delta^3(\bar{x}-\bar{x}')\delta(q-q'). \tag{3.4b}$$

We can also introduce smeared field operators. For $g \in E$ let

$$\psi(g) = \int d^3x\, dq\, g^*(\bar{x},q)\psi(\bar{x},q), \tag{3.4'a}$$

and then

$$[\psi(g_1), \psi^+(g_2)] = (g_1;g_2), \tag{3.4'b}$$

where $(\,;\,)$ is the scalar product in E.

In Sec. 2 we defined operators P^μ $M^{\mu\nu}$, and D on S in E, (2.5a)–(2.5e), which according to Theorem 1 spans a representation of $\mathfrak{w}$. We now set up the corresponding lifted operators $d\Gamma(P^\mu)$, $d\Gamma(M^{\mu\nu})$ and $d\Gamma(D)$ on the dense subspace $\Gamma(S) \subset \Gamma(E)$. Letting $|\alpha\rangle \in \Gamma(S)$, we obtain

$$d\Gamma(P^0)|\alpha\rangle = \int d^3x\, dq\, \psi^+ V^{1/2} \psi |\alpha\rangle, \tag{3.5a}$$

$$d\Gamma(\bar{P})|\alpha\rangle = \int d^3x\, dq\, \psi^+(-i\overline{\nabla})\psi|\alpha\rangle, \tag{3.5b}$$

$$d\Gamma(\bar{J})|\alpha\rangle = \int d^3x\, dq\, \psi^+(-i\bar{x}\times\overline{\nabla})\psi|\alpha\rangle, \tag{3.5c}$$

$$d\Gamma(\bar{K})|\alpha\rangle = \int d^3x\, dq\, \psi^+(-V^{1/2}\bar{x} - \tfrac{1}{2}V^{-1/2}\overline{\nabla})\psi|\alpha\rangle, \tag{3.5d}$$

$$d\Gamma(D)|\alpha\rangle = \int d^3x\, dq\, \psi^+ \frac{i}{2}$$

$$\times(\bar{x}\overline{\nabla} + \overline{\nabla}\bar{x} + q\partial_q + \partial_q q)\psi|\alpha\rangle. \tag{3.5e}$$

Theorem 3: The operators (3.5a)–(3.5e) are exactly the operators, (2.5a)–(2.5e) lifted to Fock space.

Proof: The operators (3.5a)–(3.5e) do not change particle number. Hence it is enough to consider their properties on the n-particle sectors $S^{(n)} \subset E^{(n)}$. Furthermore, we can limit ourselves to the set of vectors $|\alpha\rangle = \psi^+(g_1)\cdots\psi^+(g_n)|0\rangle$ with $g_i \in S^{(1)}$ since these span $S^{(n)}$. Then let $|\beta\rangle = \psi^+(f_1)\cdots\psi^+(f_n)|0\rangle$ with $f_i \in E^{(1)}$. Then using (3.4b) and

$$V^{1/2}(\bar{x},q)\delta^3(\bar{x}-\bar{x}')\delta(q-q') = V^{1/2}(\bar{x}',q')\delta^3(\bar{x}-\bar{x}')\delta(q-q'), \tag{3.6}$$

we obtain

$$\langle\beta|\,d\Gamma(P^0)\,|\alpha\rangle = \sum_{\text{perm}} (f_{i_1}; V^{1/2} g_{j_1})(f_{i_2};g_{j_2})\cdots(f_{i_n};g_{j_n}), \tag{3.7}$$

where the sum is over permutations of $i_1,\ldots,i_n$ and $j_1,\ldots,j_n$. Hence it is obvious that $d\Gamma(P^0)$ is exactly the operator P^0 in (2.5a) lifted to the Fock space $\Gamma(E)$. The other operators can be treated in a similar way and it is obvious that the operators (3.5a)–(3.5e) fulfill a theorem corresponding to theorem 1. Q.E.D.

The next step in our construction will be to set up a Lagrangian free-field theory which in form will be very close to the representation (2.10a)–(2.10e) of $\mathfrak{w}$ in $\mathscr{H}(x^0)$. We introduce fields $\Phi(x,q)$ as follows:

$$\Phi(x,q) = \Phi^{(+)}(x,q) + \Phi^{(-)}(x,q)$$
$$= G(x^0)\psi(\bar{x},q) + G(-x^0)\psi^+(\bar{x},q), \tag{3.8a}$$

so that

$$\Phi^{(+)}(x,q) = \sum_k \int d^3p\, (2\pi)^{-3/2}\pi^{-1/2}$$

$$\times \exp[-i(\bar{p}^2 + m_0^2 k^2)^{1/2}x^0 + i\bar{p}\bar{x}]$$

$$\times(\bar{p}^2 + m_0^2 k^2)^{-1/4} a_k(\bar{p}) \tag{3.8b}$$

and

$$\Phi^{(-)}(x,q)=[\Phi^{(+)}(x,q)]^*. \tag{3.8c}$$

We also introduce conjugate fields $\pi(x,q)$

$$\pi(x,q)=\dot{\Phi}(x,q)=\pi^{(+)}(x,q)+\pi^{(-)}(x,q)$$
$$=-iV^{1/2}G(x^0)\psi(\bar{x},q)+iV^{1/2}G(-x^0)\psi^*(\bar{x},q) \tag{3.9}$$

The fields Φ and π fulfill canonical commutation relations (CCR)

$$[\Phi(x^0,\bar{x},q),\pi(x^0,\bar{x}',q')]=-i\delta^3(\bar{x}-\bar{x}')\delta(q-q'), \tag{3.10}$$

and the fields $\Phi(x,q)$ satisfy a generalized Klein–Gordon field equation of the same form as the wave equation (2.11) in $\mathscr{H}(x^0)$,

$$(\Box-m_0^2\partial_q^2)\Phi(x,q)=0. \tag{3.11}$$

This field equation can be derived via a variation principle from an action integral

$$I[\Phi]=\int d^4x\,dq\ \mathscr{L}_0, \tag{3.12a}$$

where

$$\mathscr{L}_0=\tfrac{1}{2}(\partial_\mu\Phi)^2-\tfrac{1}{2}m_0^2(\partial_q\Phi)^2. \tag{3.12b}$$

This action is locally invariant under $\mathfrak{w}$, i.e., it is invariant under infinitesimal $\mathfrak{w}$-transformations but not necessarily under finite $\mathfrak{w}$-transformations. Guided by Noether's theorem (which, however, is not valid here, at least not in the usual formulation), we can set up the following representation of the generators of the Weyl algebra:

$$P_L^0=:\int d^3x\,dq\ [\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q\Phi)^2]:, \tag{3.13a}$$

$$\bar{P}_L=:\int d^3x\,dq\,\pi(-\bar{\nabla})\Phi:, \tag{3.13b}$$

$$\bar{J}_L=:\int d^3x\,dq\,\pi(-\bar{x}\times\bar{\nabla})\Phi:, \tag{3.13c}$$

$$\bar{K}_L=:\int d^3x\,dq$$
$$\times\{-\bar{x}\,[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q\Phi)^2]$$
$$-x^0\pi\bar{\nabla}\Phi\}:, \tag{3.13d}$$

$$D_L=:\int d^3x\,dq\,\{x^0\,[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q\Phi)^2]$$
$$+\pi(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{3}{2})\Phi\}:. \tag{3.13e}$$

We shall now prove that the operators (3.13a)–(3.13e) fulfill the commutation relations of $\mathfrak{w}$, first in a straightforward but formal way (Theorem 4), and then by explicitly and in detail showing that the operators P_L^μ, $M_L^{\mu\nu}$, and D_L in (3.13a)–(3.13e) are identical to the operators $d\Gamma(P^\mu)$, $d\Gamma(M^{\mu\nu})$, and $d\Gamma(D)$ in (3.5a)–(3.5e) in $\Gamma(E)$ (Theorem 5).

Theorem 4: Assume that partial integrations can be performed as often as needed and that outintegrated terms vanish. It can then be proven that P_L^μ, $M_L^{\mu\nu}$, and D_L in (3.13a)–(3.13e), evaluated at the same time x^0, fulfill the commutation relations of $\mathfrak{w}$.

Proof: The normal ordering changes the operators only by an additive constant. Hence we can neglect the normal ordering in this proof since such constants do not affect the commutators.

We start by considering the commutator between D_L and Φ at equal times. Using the CCR (3.10), we find

$$[D_L(x^0),\Phi(x^0,\bar{x},q)]$$
$$=-i\int d^3x'\,dq'\,\delta^3(\bar{x}-\bar{x}')\delta(q-q')$$
$$\times[x^0\pi(x^0,\bar{x}',q')+(\bar{x}'\bar{\nabla}'+q'\partial_{q'}+\tfrac{3}{2})\Phi(x^0,\bar{x}',q')]$$
$$=-i(x^\mu\partial_\mu+q\partial_q+\tfrac{3}{2})\Phi(x,q). \tag{3.14}$$

Performing partial integration (cf. the assumption in the theorem) and using the field equation (3.11), we obtain for the commutator with π

$$[D_L(x^0),\pi(x^0,\bar{x},q)]$$
$$=i\int d^3x'\,dq'\{x^0(\bar{\nabla}'\Phi\bar{\nabla}'+m_0^2\partial_{q'}\Phi\partial_{q'})$$
$$+\pi(\bar{x}'\bar{\nabla}'+q'\partial_{q'}+\tfrac{3}{2})\}\delta^3(\bar{x}-\bar{x}')\delta(q-q')$$
$$=-i[x^0(\bar{\nabla}^2+m_0^2\partial_q^2\Phi+(\bar{\nabla}\bar{x}+\partial_q q-\tfrac{3}{2})\pi]$$
$$=-i(x^\mu\partial_\mu+q\partial_q+\tfrac{5}{2})\pi. \tag{3.15}$$

Utilizing (3.14) and (3.15), we can now consider the commutation relation between D_L and P_L^0:

$$[D_L(x^0),P_L^0(x^0)]$$
$$=-i\int d^3x\,dq[\pi(x^\mu\partial_\mu+q\partial_q+\tfrac{5}{2})\pi$$
$$+\bar{\nabla}\Phi(x^\mu\partial_\mu+q\partial_q+\tfrac{5}{2})\bar{\nabla}\Phi$$
$$+m_0^2\partial_q\Phi(x^\mu\partial_\mu+q\partial_q+\tfrac{5}{2})\partial_q\Phi]$$
$$=-i\int dx^3\,dq$$
$$\times[x^0\pi(\bar{\nabla}^2+m_0^2\partial_q^2)\Phi+x^0\pi(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{5}{2})\pi$$
$$+\bar{\nabla}\Phi(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{5}{2})\bar{\nabla}\Phi+x^0m_0^2\partial_q\Phi\partial_q\pi$$
$$+m_0^2\partial_q\Phi(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{5}{2})\partial_q\Phi]. \tag{3.16}$$

This last expression is simplified by partial integration. We then obtain

$$
\begin{aligned}
&[D_L(x^0),P_L^0(x^0)] \\
&\quad = -i\int d^3x\,dq \\
&\qquad \times[-x^0\bar{\nabla}\pi\,\bar{\nabla}\Phi - x^0 m_0^2\partial_q\pi\,\partial_q\Phi + \tfrac{1}{2}x^0\bar{x}\,\bar{\nabla}\pi^2 \\
&\qquad + \tfrac{1}{2}x^0(\bar{x}\,\bar{\nabla}+q\partial_q+\tfrac{5}{2})\pi^2 + x^0\bar{\nabla}\Phi\bar{\nabla}\pi \\
&\qquad + \tfrac{1}{2}(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{5}{2})(\nabla\Phi)^2 \\
&\qquad + m_0^2\partial_q\Phi\,\partial_q\pi + \tfrac{1}{2}m_0^2(\bar{x}\,\bar{\nabla}+q\partial_q+\tfrac{5}{2})(\partial_q\Phi)^2] \\
&\quad = -i\int d^3x\,dq[(-\tfrac{3}{2}-\tfrac{1}{2}+\tfrac{5}{2})x^0\pi^2 \\
&\qquad + (-\tfrac{3}{2}-\tfrac{1}{2}+\tfrac{5}{2})(\bar{\nabla}\Phi)^2 \\
&\qquad + m_0^2(-\tfrac{3}{2}-\tfrac{1}{2}+\tfrac{5}{2})(\partial_q\Phi)^2] \\
&\quad = -iP_L^0(x^0). \qquad (3.17)
\end{aligned}
$$

This is in accordance with (2.2a). In a similar manner it can be proven that P_L^μ, $M_L^{\mu\nu}$, and D_L fulfils also the other commutation relations of $\mathfrak{w}$. Q.E.D.

Theorem 5: The Lagrangian operators P_L^μ, $M_L^{\mu\nu}$, and D_L, defined in (3.13a)–(3.13e), are identical with the operators $d\Gamma(P^\mu)$, $d\Gamma(M^{\mu\nu})$ and $d\Gamma(D)$, defined in (3.5a)–(3.5e).

Proof: Let the vectors $|\alpha\rangle\in S^{(n)}$ and $|\beta\rangle\in S^{(m)}$ be defined by

$$|\alpha\rangle = \psi^*(g_1)\cdots\psi^*(g_n)|0\rangle, \qquad (3.18a)$$

$$|\beta\rangle = \psi^*(f_1)\cdots\psi^*(f_m)|0\rangle, \qquad (3.18b)$$

where $g_i\in S$ and $f_i\in S$. As in the proof of Theorem 3 we shall use (3.6) and similar formulas, like, e.g.,

$$
\begin{aligned}
&(-V^{1/2}\bar{x}-V^{-1/2}\bar{\nabla})\delta^3(\bar{x}-\bar{x}')\delta(q-q') \\
&\quad = (-\bar{x}'V'^{1/2}+\bar{\nabla}'V'^{-1/2})\delta^3(\bar{x}-\bar{x}')\delta(q-q'). \qquad (3.6')
\end{aligned}
$$

Now consider the matrix element $\langle\beta|P_L^0|\alpha\rangle$. For the case $n=m$ we obtain

$$\langle\beta|P_L^0|\alpha\rangle = \sum_{\text{perm}} A_{i_1,j_1}(f_{i_1};g_{j_1})\cdots(f_{j_n};g_{j_n}), \qquad (3.19a)$$

where

$$A_{i,j} = \langle 0|\psi(f_i)P_L^0\psi^*(g_j)|0\rangle. \qquad (3.19b)$$

To evaluate (3.19b), we insert the defining expressions (3.8a) and (3.9) for Φ and π which expresses these operators in terms of ψ and ψ^*. The terms in P_L^0 which are quadratic in ψ or ψ^* do not contribute in (3.19a) and (3.19b). After performing normal ordering we find

$$
\begin{aligned}
A_{i,j} = \Big\langle 0\Big|\int f_i^*\psi d^3x\,dq\int\{&V^{1/2}G(-x^0)\psi^*V^{1/2}G(x^0)\psi \\
&+(\bar{\nabla}G(-x^0)\psi^*)(\bar{\nabla}G(x^0)\psi) \\
&+(\partial_q G(-x^0)\psi^*)(\partial_q G(x^0)\psi)\}d^3x_2\,dq_2 \\
&\times\int\psi^* g_j d^3x_3\,dq_3\Big|0\Big\rangle. \qquad (3.20)
\end{aligned}
$$

Using the commutation relation (3.4b) between ψ and ψ^*, we then obtain

$$
\begin{aligned}
A_{i,j} = \int d^3x_1\,dq_1\,d^3x_2dq_2\,d^3x_3\,dq_3 f_i^*(\bar{x}_1,q_1) \\
&\times[(V^{1/2}G(-x^0))_{\bar{x}_2,q_2}\delta^3(\bar{x}_1-\bar{x}_2) \\
&\times\delta(q_1-q_2)(V^{1/2}G(x^0))_{\bar{x}_2,q_2}\delta^3(\bar{x}_2-\bar{x}_3) \\
&\times\delta(q_2-q_3)+\cdots]g_j(\bar{x}_3,q_3). \qquad (3.21)
\end{aligned}
$$

We then use (3.6) to change variables in the differential operators in front of the δ functions and perform the integral over x_2 and q_2.

$$
\begin{aligned}
A_{i,j} = \int d^3x_1\,dq_1\,d^3x_3\,dq_3 f_i^*(\bar{x}_1,q_1) \\
&\{(V^{1/2}G(-x^0)_{\bar{x}_1,q_1}(V^{1/2}G(x^0))_{\bar{x}_1,q_1} \\
&\times\delta^3(\bar{x}_1-\bar{x}_3)\delta(q_1-q_3)+\cdots\}g_j(\bar{x}_3,q_3). \qquad (3.22)
\end{aligned}
$$

Next we perform partial integration in order to have the differential operators operating on f_i^* and g_j instead of on the δ functions. Here we observe that since $f_i, g_j\in S$ we then obtain

$$A_{i,j} = (f_i; V^{1/2}g_j). \qquad (3.23)$$

The terms in P_L^0 which are quadratic in ψ are nonvanishing, and are the only ones which are so, only when $m=n-2$, which case we shall now consider. We shall make use of the following formal identities:

$$\Phi^{(-)}(x,q) = G(x^0)\psi(\bar{x},q) = \psi(G(x^0)\delta_{\bar{x}}^3\delta_q), \qquad (3.24a)$$

$$\pi^{(-)}(x,q) = -iV^{1/2}G(x^0)\psi(\bar{x},q) = \psi(-iV^{1/2}G(x^0)\delta_{\bar{x}}^3\delta_q). \qquad (3.24b)$$

Then

$$
\begin{aligned}
\langle\beta|P_L^0|\alpha\rangle = \int d^3x\,dq\langle 0|\psi(f_1)\cdots\psi(f_{n-2}) \\
&\times\{\psi(-iV^{1/2}G(x^0)\delta_{\bar{x}}^3\delta_q)
\end{aligned}
$$

$$\times\psi(-iV^{1/2}G(x^0)\delta^3_{\vec{x}}\delta_q)+\cdots\}$$

$$\times\psi^*(g_1)\cdots\psi^*(g_n)\,|0\rangle$$

$$=\sum_{\text{perm}}\int d^3x\,dq\,(f_{i_1};g_{j_1})\cdots(f_{i_{n_1}};g_{j_{n_1}})$$

$$\times\{(-iV^{1/2}G(x^0)\delta^3_{\vec{x}}\delta_q;g_{j_{n_1+1}})$$

$$\times(-iV^{1/2}G(x^0)\delta^3_{\vec{x}}\delta_q;g_{j_{n_1+2}})+\cdots\}. \tag{3.25}$$

To simplify this expression, we first perform partial integration in the scalar products between the braces in order to move the differential operators from the δ functions to the functions g_i. The out-integrated terms vanish as before since $g_i\in S$. We then perform two integrations to eliminate the δ functions and obtain

$$\langle\beta\,|P^0_L\,|\alpha\rangle=\sum_{\text{perm}}(f_{i_1};g_{j_1})\cdots(f_{i_{n_1+2}};g_{j_{n_1+2}})$$

$$\times\{(-iV^{1/2}G(x^0)g^*_{j_{n_1+1}};-iV^{1/2}$$

$$G(x^0)g_{j_{n_1}})+\cdots\}. \tag{3.26}$$

To simplify further, we integrate partially once more and, after using the defining identity $V=-\Delta-\partial_q^2$, we find that the matrix element vanishes in the case $m=n-2$.

In the case $m>n$ the only possibly nonvanishing terms in $\langle\beta\,|P^0_L\,|\alpha\rangle$ are those which are quadratic in ψ^* and they contribute only when $m=n+2$. It can, however, be proven, in a similar way as before, that the matrix element vanishes also in this case.

Inserting (3.26) in (3.19a), we conclude that

$$\langle\beta|P^0_L\,|\alpha\rangle$$

$$=\begin{cases}\sum_{\text{perm}}(f_{i_1};V^{1/2}g_{j_1})(f_{i_2};g_{j_2})\cdots(f_{i_n};g_{j_n}), & \text{if } m=n,\\ 0, & \text{if } m\neq n.\end{cases} \tag{3.27}$$

Comparing (3.27) with (3.7) we find that $P^0_L=d\Gamma(P^0)$. The other operator identities in the theorem can be proven in a similar way. Q.E.D.

This theorem shows that the assumption in Theorem 4 are reasonable.

4. SCATTERING OF MODEL PARTICLES

In this section we introduce dynamics into the model by adding an interaction term, which is locally invariant under $\mathfrak{w}$, to the action (3.12a). Let (for simplicity)

$$\mathcal{L}_I=-\lambda q^{n_0}(\partial_q^{n_1}\Phi)(\partial_q^{n_2}\Phi)(\partial_q^{n_3}\Phi). \tag{4.1a}$$

Then the contribution from (4.1a) to the action is $\mathfrak{w}$-invariant if

$$n_0=n_1+n_2+n_3-\tfrac{1}{2},\quad \text{for } n_{1,2,3}=0,1,2,3,\cdots \tag{4.1b}$$

since then the action has no scale dimension.

From the total action we derive the following field equation for the interacting field:

$$(\Box-m_0^2\partial_q^2)\Phi=-\lambda(-1)^{n_1}\partial_q^{n_1}[q^{n_0}\partial_q^{n_2}\Phi\partial_q^{n_3}\Phi]$$

$$-\lambda(-1)^{n_2}\partial_q^{n_2}[q^{n_0}\partial_q^{n_1}\Phi\partial_q^{n_2}\Phi]$$

$$-\lambda(-1)^{n_3}\partial_q^{n_3}[q^{n_0}\partial_q^{n_1}\Phi\partial_q^{n_2}\Phi]. \tag{4.2}$$

Guided by Noether's theorem applied on the total action, we obtain the following generators:

$$P^0_L=:\int d^3x\,dq[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q^n\Phi)^2$$

$$+\lambda q^{n_0}\partial_q^{n_1}\Phi\partial_q^{n_2}\Phi\partial_q^{n_3}\Phi]:, \tag{4.3a}$$

$$\bar{P}_L=:\int d^3x\,dq\,\pi(-\bar{\nabla})\Phi:, \tag{4.3b}$$

$$\bar{J}_L=:\int d^3x\,dq\,\pi(-\bar{x}\times\bar{\nabla})\Phi:, \tag{4.3c}$$

$$\bar{K}_L=:\int d^3x\,dq\{-\bar{x}[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q\Phi)^2$$

$$+\lambda q^{n_0}\partial_q^{n_1}\Phi\partial_q^{n_2}\Phi\partial_q^{n_3}\Phi]-x^0\pi\bar{\nabla}\Phi\}:, \tag{4.3d}$$

$$D_L=:\int d^3x\,dq\{x^0[\tfrac{1}{2}\pi^2+\tfrac{1}{2}(\bar{\nabla}\Phi)^2+\tfrac{1}{2}m_0^2(\partial_q\Phi)^2$$

$$+\lambda q^{n_0}\partial_q^{n_1}\Phi\partial_q^{n_2}\Phi\partial_q^{n_3}\Phi]$$

$$+\pi(\bar{x}\bar{\nabla}+q\partial_q+\tfrac{3}{2})\Phi\}:. \tag{4.3e}$$

Theorem 6: Assume as in Theorem 4 that partial integration can be performed as often as needed and that outintegrated terms vanish. Then it can be proven that P^μ_L, $M^{\mu\nu}_L$, and D_L as defined in (4.3a)–(4.3e) fulfill the commutation relations of $\mathfrak{w}$.

Proof: The theorem is proved in the same way as Theorem 3.

Next we shall study scattering and calculate S-matrix elements and cross sections. We recall that in the noninteracting case we have set up representations (3.5a)–(3.5e) of $\mathfrak{w}$ on the subspace $\Gamma(S)\subset\Gamma(E)$. Here we note that the Poincaré part of the representations are not integrable to a representation of the Poincaré group on these subspaces. However, on $\Gamma((R^3)\otimes C(T)^\infty_{0,2,4\cdots})\subset\Gamma(E)$ the Poincaré generators are in-

tegrable. We shall now stay in the Poincaré integrable domains and turn to the study of the S-matrix. Perturbation theory can be brought over to this case with minor changes and the deductions are very similar to those in the usual case (see e.g., Ref. 7).

First we shall make some changes towards a more manifest covariance. We change to a new normalization of the states. Let

$$|\bar{p},k\rangle_c=(\omega_k(\bar{p}))^{1/2}|\bar{p},k\rangle, \tag{4.4a}$$

and hence

$${}_c\langle\bar{p},k|\bar{p}',k'\rangle_c=\omega_k(\bar{p})\delta^3(\bar{p}-\bar{p}')\delta_{kk'}. \tag{4.4b}$$

Let $b_k^+(\bar{p})$ and $b_k(\bar{p})$ be the creation and annihilation operators associated with these states. Then

$$b_k(\bar{p})=(\omega_k(\bar{p}))^{1/2}a_k(\bar{p}), \tag{4.5}$$

where $a_k(\bar{p})$ is the annihilation operator of the state $|\bar{p},k\rangle$. We also have

$$\Phi^{(+)}(x,q)=\sum_k\int\frac{d^3p}{\omega_k(\bar{p})}(2\pi)^{-3/2}\pi^{-1/2}$$

$$\times\exp[-i\omega_k(\bar{p})x^0+i\bar{p}\bar{x}]\sin kq\, b_k(\bar{p}). \tag{4.6}$$

This is in complete analogy with Ref. 4, Eq. (7:72a).

The following reduction formula can be derived (cf., e.g., Ref. 7):

$${}_c\langle\bar{p}_1,k_1;\ldots;\text{out}|\bar{p}'_1,k'_1;\ldots;\text{in}\rangle_c$$

$$=i^{m+n}\prod_{i=1}^{n}\prod_{j=1}^{m}\int d^4x_i\,dq_i d^4x'_j\,dq'_j$$

$$\times(2\pi)^{-3/2}\pi^{-1/2}\,e^{ip_ix_i}\sin kq(\overrightarrow{\Box_{x_i}-m_0^2\partial_{q_i}^2})$$

$$\times\langle0|T(\Phi(x_1,q_1)\cdots)|0\rangle(\overleftarrow{\Box_{x_j}-m_0^2\partial_{q'_j}^2})(2\pi)^{-3/2}\pi^{-1/2}$$

$$\times e^{-ip'_jx'_j}\sin k'_jq'_j. \tag{4.7}$$

The expression for the τ-functions will be

$$\tau(x_1,q_1;\cdots)$$

$$\equiv\langle0|T(\Phi(x_1;q_1)\cdots)|0\rangle$$

$$=\frac{\langle0|T(\Phi_{\text{in}}(x_1,q_1)\cdots\exp[-i\int_{-\infty}^{\infty}dt\,H_I(\Phi_{\text{in}},\pi_{\text{in}})])|0\rangle}{\langle0|T(\exp[(-i\int_{-\infty}^{\infty}dt\;H_I(\Phi_{\text{in}},\pi_{\text{in}})])|0\rangle}. \tag{4.8}$$

Wick's theorem will be as usual and only connected graphs contribute. The propagator will be

$$\langle0|T(\Phi_{\text{in}}(x_1,q_1)\Phi_{\text{in}}(x_2,q_2))|0\rangle$$

$$=i\Delta_F(x_1-x_2;q_1-q_2)$$

$$=\frac{i}{(2\pi)^4}\frac{2}{\pi}\sum_{k=1}^{\infty}\int d^4p\,\frac{1}{p^2-m_0^2k^2+i\epsilon}$$

$$\times e^{-ip(x_1-x_2)}\sin kq_1\sin kq_2. \tag{4.9}$$

All these formulas can be summarized in the following Feynman rules:

(1) For each in-line write $(2\pi)^{-3/2}\pi^{-1/2}e^{-ip_ix_i}\sin k'_iq'_i$.

(2) For each out-line write $(2\pi)^{-3/2}\pi^{-1/2}e^{ip'_jx'_j}\sin k'_jq'_j$.

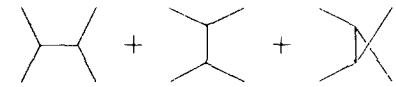
(3) For each internal line write $i\Delta_F(x_1-x_2;\,q_1-q_2)$.

(4) For each vertex write
$(-i\lambda)\int d^4x\,dq\;q^{n_0}\partial_q^{n_1}(\cdots)\partial_q^{n_2}(\cdots)\partial_q^{n_3}(\cdots)$.

As an example we shall now consider two-body scattering and calculate S-matrix elements to second order. Let

$$S_{fi}^{(2)}=\langle\bar{p}_3,k_3;\;\bar{p}_4,k_4;\,\text{out}\,|\bar{p}_1,k_1;\;\bar{p}_2,k_2;\;\text{in}\rangle=I+R_{fi}^{(2)}. \tag{4.10}$$

Then

$R_{fi}^{(2)}=$ 

$$=R_{fi}^{(2)}(s)+R_{fi}^{(2)}(t)+R_{fi}^{(2)}(u)$$

$$=\sum_{\substack{\text{perm}\\ n_i\&n_i}}\{-2^{-5}\pi^{-8}\lambda^2\delta^4(p_f-p_i)$$

$$\times\int\int dq\,dq'q^{n_0}q'^{n_0}\partial_q^{n_1}\sin k_4q$$

$$\times\partial_q^{n_2}\sin k_3q\partial_{q'}^{n_1}\sin k_2q'$$

$$\times\partial_{q'}^{n'_2}\sin k_1q'\partial_q^{n_1}\partial_{q'}^{n'_1}[G(s;q,q')$$

$$+G(t;q,q')+G(u;q,q')]\}, \tag{4.11a}$$

where

$$G(z;q,q')=\sum_{k=1}^{\infty}\frac{\sin kq\sin kq'}{z-m_0^2k^2}, \tag{4.11b}$$

and where p_f is the sum of the 4-momenta in the final state and p_i is the sum of initial 4-momenta. s, t, and u are the well-known Mandelstam variables.

Using the following formulas[8]

$$\sum_{k=1}^{\infty}\frac{\cos kx}{k^2-\alpha^2}=\frac{1}{2\alpha^2}-\frac{\pi\cos\alpha(\pi-x)}{2\alpha\sin\alpha\pi}\quad(0\leqslant x\leqslant\pi), \tag{4.12a}$$

$$\sum_{k=1}^{\infty}\frac{\cos kx}{k^2+\alpha^2}=\frac{\pi\cosh\alpha(\pi-x)}{2\alpha\sinh\alpha\pi}-\frac{1}{2\alpha^2}\quad(0\leqslant x\leqslant\pi), \tag{4.12b}$$

we can sum up (4.11b) and obtain

$$G(z;q,q')=\begin{cases}\dfrac{\pi\sin[(z/m_0^2)^{1/2}(\pi-q)]\,\sin[(z/m_0^2)^{1/2}q']}{2m_0^2(z/m_0^2)^{1/2}\sin[(z/m_0^2)^{1/2}\pi]} & (z>0),\\ \dfrac{\pi-q'}{2m_0^2} & (z=0),\\ \dfrac{\pi\sinh[(-z/m_0^2)^{1/2}(\pi-q)]\,\sinh[(-z/m_0^2)^{1/2}q']}{2m_0^2(-z/m_0^2)^{1/2}\sinh[(-z/m_0^2)^{1/2}\pi]} & (z<0).\end{cases} \tag{4.13}$$

This expression is valid when $0<q'<q<\pi$. The values of $G(z;q,q')$ when $0<q<q'<\pi$ are obtained from the same expression but with q and q' interchanged.

Inserting (4.13) in (4.11), we obtain an expression for $R_{fi}^{(2)}$ which can be useful, especially when one is interested in asymptotic behavior, e.g., $s\to\infty$, $t=0$. In the low-energy region, it is, however, probably more convenient not to sum up the propagator expressions but instead perform the q and q' integrations first to obtain weights on the terms in the propagator sum. We then get

$$R_{fi}^{(2)}=\sum_{\text{perm}}\Big\{-2^{-5}\pi^{-8}\lambda^2\delta^4(p_f-p_i)\sum_{k=1}^{\infty}F_{k,k,,k}\,F_{k,k,,k}\times\Big(\frac{1}{s-m_0^2k^2}+\frac{1}{t-m_0^2k^2}+\frac{1}{u-m_0^2k^2}\Big)\Big\}, \tag{4.14a}$$

where

$$F_{k_1,k_2,k_3}=\int_0^{\pi}dq\,q^{n_0}\partial_q^{n_1}\sin k_1q\;\partial_q^{n_2}\sin k_2q\;\partial_q^{n_3}\sin k_3q. \tag{4.14b}$$

The integral (4.14b) cannot be explicity solved since n_0 is always half-odd. One can express the integral in the incomplete Γ function (where the arguments will be imaginary), but this does not help us very much. However, by expanding F in an asymptotic series in powers of $1/k$ (for $k\to\infty$) and using Riemann and Lebesgue's lemma one can derive the asymptotic behavior of the weight functions F. For small k some other approximation scheme must be used. In this way one can, in models of this kind, calculate $R_{fi}^{(2)}$ and then scattering cross sections. These quantities can then be compared with the appropriate data to discriminate between different models and different interactions.

Before we proceed, we observe that the propagator sum in (4.14a) has single poles at $z=m_0^2k^2$ $(k=1,2,3,\cdots)$ and hence $R_{fi}^{(2)}(s,t,u)$ has the same singularities. Accidentally in this model there happens to be a pole exactly at the kinematical threshold in the s channel (i.e., $s=4m_0^2$), which is awkward. This is due to the fact that this model is chosen for simplicity and will not occur in more refined models with more realistic mass spectra, or by choosing other boundary conditions for the mass spectrum problem which was treated in Sec. 2. We shall now exemplify the discussion above, studying the interaction with $\mathcal{L}_I=-\lambda q^{-1/2}\Phi^3$ and specializing to the case $k_1=k_2=k_3=k_4=1$. We shall only consider the asymptotic behavior in the limit $s\to\infty$, $t=0$. (4.11a) with (4.13) inserted will for this case be

$$\begin{aligned}R_{fi}^{(2)}&=-2^{-5}\pi^{-8}\lambda^2\delta^4(p_f-p_i)2\int_D\int dq\,dq'\,q^{-1/2}q'^{-1/2}\sin^2q\,\sin^2q'\\&\times\Big(\frac{\pi\sin[(s/m_0^2)^{1/2}(\pi-q)]\,\sin[(s/m_0^2)^{1/2}q']}{2m_0^2(s/m_0^2)^{1/2}\sin[s/m_0^2)^{1/2}]}+\frac{(\pi-q')q}{2m_0^2}\\&+\frac{\pi\sinh[(-u/m_0^2)^{1/2}(\pi-q)]\,\sinh[(-u/m_0^2)^{1/2}q']}{2m_0^2(-u/m_0^2)^{1/2}\sinh[(-u/m_0^2)^{1/2}\pi]}\Big),\end{aligned} \tag{4.15}$$

where D is the triangle in the qq' plane spanned by the points (0,0), $(\pi,0)$, and $(\pi\pi)$. The s-depending term in (4.15) is best expanded in an asymptotic series in powers of $s^{-1/2}$ (when $s\to\infty$) by integrating partially and using Riemann and Lebesgue's lemma to neglect higher terms. The first term in this expression will be proportional to s^{-1} and the second proportional to $s^{-3/2}\cot(s/m_0^2)^{1/2}$. The singularities in the second term are due to the fact that the mass eigenstates are sharp. In higher orders of perturbation theory we expect that the singularities in the second, i.e., those in the factor $\cot(s/m_0^2)^{1/2}$, will vanish. Hence we assume that the second term is nonleading.

Since we have chosen $t=0$, the t term will be proportional to a constant.

Finally we consider the u term. There we approximate $\sinh[(-u/m_0^2)^{1/2}a]$ with $\exp[(-u/m_0^2)^{1/2}a]$ when $u\to\infty$. The resulting integrals cannot be calculated explicitly, but as before we can expand them in an asymptotic series by using partial integration. The leading term will be proportional to a constant.

Since the leading terms in the t and u terms do not cancel, we obtain

$$R_{fi}^{(2)}\cong\text{const}\,\lambda^2\delta^4(p_f-p_i)\quad(s\to\infty,t=0), \tag{4.16}$$

Hence, in this limit, we obtain for the scattering cross section

$$\sigma_{\text{el}}\cong\lambda^4s^{-1}. \tag{4.17}$$

As a second example we will study the interaction with $\mathcal{L}_I=-\lambda q^{11/2}(\partial_q^2\Phi)^3$. Then using (4.11) the R matrix will be, if we specialize to $k_1=k_2=k_3=k_4=1$,

$$R_{fi}^{(2)}=-2^{-5}\pi^{-6}\lambda^2\delta^4(p_f-p_i)$$

$$\times \int_0^\pi \int_0^\pi dq\, dq'\, q^{11/2} q'^{11/2} \sin^2 q \sin^2 q'$$

$$\times [G_1(s; q,q') + G_1(t; q,q') + G_1(u; q,q')], \qquad (4.18a)$$

where

$$G_1(z; q,q') = \sum_{k=1}^{\infty} \frac{k^4 \sin kq \sin kq'}{z - m_0^2 k^2}$$

$$= (m_0^{-2} \partial_q^2 + z)\delta(q-q') + z^2 G(z; q,q'). \qquad (4.18b)$$

When the insert (4.18b) in (4.18a), the first term in (4.18b) will only give rise to a constant since we can use the well-known identity $s+t+u=4m_0^2$ to eliminate z. Then we can calculate the other terms in a similar manner as in the first example. We obtain that the leading term in the s term will be proportional to s. The t term will naturally be a constant since we consider only $t=0$. Finally the u term will give a term proportional to u^2 and this term will dominate the behavior of the R matrix when $s \to \infty$ and $t=0$, i.e.,

$$R_{fi}^{(2)} \cong \text{const} \lambda^2 \delta^4(p_f - p_i) u^2, \qquad (4.19)$$

and the cross section will in this limit be

$$\sigma_{\text{el}} \cong \text{const} \lambda^4 s^3. \qquad (4.20)$$

4. DISCUSSION

We begin by clarifying some properties in the construction of our model. This model is based on local Weyl algebra symmetry. This symmetry is local in the sense that the model is based on a representation of the Weyl algebra that cannot be exponentiated to a representation of the Weyl group. The representation of $\mathfrak{w}$ in $\mathscr{H}(x^0)$ was verified on the subspace $S(x^0)$. This subspace is not invariant under the action of the generators of $\mathfrak{w}$, for instance it is then not invariant under time development. Hence, to detect the Weyl algebra symmetry of the system we must prepare a state [belonging to $S(x^0)$] and perform the measurements at the same time. However, if we prepare the system in a state belonging to the subspace $\mathscr{S}(R^3) \otimes C(T)_{0,2,4,\ldots}^{\infty}$ in $\mathscr{H}(x^0)$, we have full Poincaré group symmetry since the system stays in this subspace under Poincaré transformations since this subspace is invariant under the action of the Poincaré generators.

One could argue that a model like the one discussed in this paper is not possible, according to the no-go theorem of Coleman–Mandula.[9] They, however, only mention a case like ours in a footnote and seem not to have observed the possibility of two domains of definition, i.e., one on which the nonintegrable Weyl algebra symmetry is realized and another on which the Poincaré algebra is integrable. Indeed, in our model the operator D_L in (4.3e) does not satisfy Lemma 1 of Ref. 9.

The model described in this paper is intended as a first example of a new class of models, and we have primarily been interested in showing that it is indeed possible to construct such a model, in what sense it is possible, and how it can be done.

Now that these problems have been clarified it can be interesting to study the renormalizability of this type of models, self-energy corrections, etc. It is also natural to ask for a more realistic model. Such a model could, for instance, involve a representation of $\mathfrak{w}$ with an infinite multiplet of fermions (with different masses) coupled to a representation with an infinite multiplet of bosons (and to the electromagnetic field etc.) Representations of this kind, which might be adapted to a model of this kind, have indeed recently been found by one of us.[10]

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Summation of partial wave expansions in the scattering by long range potentials. II. Numerical applications[a)]

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The numerical application of a sequence transformation method proposed in a previous work is considered for the calculation of differential cross-sections corresponding to processes where long range interactions are important. The advantages of the approach, as a summation algorithm for the partial wave expansion of the scattering amplitude, are shown for the cases of scattering by the Lennard–Jones, repulsive inverse square, and Coulombic potentials, and for the scattering of electrons by helium in the intermediate energy range. Furthermore, the method proves to be a regularizing procedure for divergent and oscillating partial wave expansions.

1. INTRODUCTION

Most of the interactions proposed to explain atomic and molecular collision phenomena are of the long-range type. Because of this fact, and depending on the particular process and of the energy involved, there may be an important contribution of the high order phase shifts in the partial wave expansion of the scattering amplitude. When this is the case, the latter is poorly convergent and can even be divergent or oscillating.

There are various methods able to deal with some of these situations, based on semiclassical approximations.[1] However, an interesting approach is to formulate a general calculation scheme, which avoids physical approximations and intends to resume efficiently the available quantum information. With this purpose, the Punctual Padé Approximants were introduced in a previous paper.[2] A set of theorems were proven regarding their asymptotic rate of convergence, when summing the partial wave expansions of the scattering amplitude and total cross section, corresponding to long-range potentials. In this work, we deal with a numerical study of the method, showing its practical importance. In Sec. 2 an outline is made of the approach, and its particular use in the case of scattering problems is considered in Sec. 3. Numerical applications in the calculation of elastic differential cross sections, corresponding to the scattering by usual potentials in atomic and molecular collision processes, are described in Sec. 4, while the general discussion of the results is given in Sec. 5.

2. TRANSFORMATION OF SERIES AND SEQUENCES

Consider the formal infinite sum

$$C(1)=\sum_{r=0}^{\infty} b_r \tag{2.1}$$

and its associated infinite sequence of partial sums $\{C_m\}$, defined by

$$C_m=\sum_{r=0}^{m} b_r. \tag{2.2}$$

Clearly, (2.1) can be seen as a particular case of the power series

$$C(z)=\sum_{r=0}^{\infty} b_r z^r \tag{2.3}$$

corresponding to $z=1$. Conversely, a formal expansion (2.3) can be associated to any given infinite sequence $\{C_m\}$, by defining $b_0=C_0$ and $b_m=C_m-C_{m-1}$ for $m\geqslant 1$. This equivalence allows one, in principle, to consider power series summation methods and procedures intended to approximate the limiting values of sequences, without further distinction.

In order to deal with slowly convergent or divergent sequences $\{C_m\}$, Shanks[3] introduced the nth order $E_n(C_m)$ transformation. It is nonlinear, and defined as a formal generalization of Aitken's Δ^2-extrapolation formula, which corresponds to $n=1$. The Δ^2 scheme can be interpreted geometrically in a two-dimensional space as a linear extrapolation involving the vectors $(C_{m+k},\ C_{m+k+1})$ with $k=0,1$. Likewise, it is possible to visualize $E_n(C_m)$ as an hyperplane extrapolation in a $(n+1)$-dimensional space, involving the vectors $(C_{m+k},\ C_{m+k+1},\ \ldots,\ C_{m+k+n})$ with $k=0,1,\ldots n$.[4] Furthermore, it can be shown that these transformations are simply related with the Padé approximations (PA) to the series $C(z)$,[5] by

$$E_n(C_m)=[n,n+m]_{C(1)}, \tag{2.4}$$

where $[n,n+m]_{C(1)}$ is the Punctual Padé Approximant (PPA) to the power series (2.3), for $z=1$. In this way, one has a new interpretation for the approximants in the Padé table. Its nth row, composed by the $[n,n+m]$ with fixed n, can be viewed as an nth order Shanks' transformation of the original sequence $[0,m]=C_m$, i.e., of the first row the table.

Like PA, the $E_n(C_m)$ are given in a compact form by determinantal quotients, not readily computable for large n. To overcome this difficulty Wynn[6] proposed the ϵ algorithm, which allows for a recursive calculation of the $E_n(C_m)$. In this scheme, a table of magnitudes $\epsilon_n^{(m)}$ is generated with the recurrence formula

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$$\epsilon_{n+1}^{(m)}=\epsilon_{n-1}^{(m+1)}+(\epsilon_n^{(m+1)}-\epsilon_n^{(m)})^{-1} \tag{2.5}$$

and the boundary values $\epsilon_{-1}^{(m)}=0$, $\epsilon_0^{(m)}=C_m$. Then, one has

$$\epsilon_{2n}^{(m)}=E_n(C_m),$$

while the $\epsilon_{2n+1}^{(m)}$ are auxiliary quantities without any direct meaning. By successive application of (2.5), and eliminating the $\epsilon_{2n+1}^{(m)}$, Wynn found the so called "missing identity of Frobenius"[5,7]:

$$\begin{aligned}&([n+1,m]-[n,m])^{-1}-([n,m]-[n-1,m])^{-1}\\&\quad=([n,m+1]-[n,m])^{-1}-([n,m]-[n,m-1])^{-1},\end{aligned} \tag{2.6}$$

which allows one to generate the Padé table recurrently, starting with the boundary conditions $[0,m]=C_m$, $[-1,m]=\infty$, and $[n,-1]=0$.

The main difficulty in the use of Eq. (2.5) and (2.6) arises when reaching convergence, and comes from the presence of small differences in the denominators. A more stable variant, from the computational point of view, is Bauer's η algorithm.[8] It is nonlinear series transformation working only with the coefficients b_r of the series (2.1). In this scheme, one constructs the table

$$\begin{array}{ccccccc}\eta_0^0 & & & & & & \\ & \eta_1^0 & & & & & \\ \eta_0^1 & & \eta_2^0 & & & & \\ & \eta_1^1 & & \eta_3^0 & & & \\ \eta_0^2 & & \eta_2^1 & & \eta_4^0 & \cdots & \\ & \eta_1^2 & & \eta_3^1 & \vdots & & \\ \eta_0^3 & & \eta_2^2 & \vdots & \vdots & & \\ \vdots & \eta_1^3 & \vdots & \vdots & & & \\ & \vdots & \vdots & & & & \end{array} \tag{2.7}$$

by using the recurrence formulas

$$\begin{aligned}&\eta_{2n+1}^{m}=\eta_{2n}^{m+1}-\eta_{2n}^{m}+\eta_{2n-1}^{m+1},\\&(\eta_{2n+2}^{m})^{-1}=(\eta_{2n+1}^{m+1})^{-1}-(\eta_{2n+1}^{m})^{-1}+(\eta_{2n}^{m+1})^{-1},\end{aligned} \tag{2.8}$$

with the initial values $\eta_0^m=\infty$ and $\eta_1^m=b_m$. Then,

$$\begin{aligned}&E_n(C_m)=[n,n+m]_{C(1)}=\sum_{k=0}^{m-1}\eta_1^k+\sum_{k=1}^{2n+1}\eta_k^m,\\&E_{n+1}(C_{m-1})=[n+1,n+m]_{C(1)}\\&\qquad=\sum_{k=0}^{m-1}\eta_1^k+\sum_{k=1}^{2n+2}\eta_k^m,\end{aligned} \tag{2.9}$$

where the first sum should be omitted when $m=0$, and $C_{-1}=0$. It should be noted that when the so-called forward application of the algorithm is considered, it is sufficient to store the last determined upper sloping diagonal of the array (2.7). Furthermore, inspection of Eqs. (2.8) and (2.9) shows that when calculating $[n,n+m]_{C(1)}$, the information contained in the first m terms of the series $C(1)$ (or of the first m members of the sequence $\{C_m\}$) is resumed in

$$C_{m-1}=\sum_{k=0}^{m-1}\eta_1^k=\sum_{k=0}^{m-1}b_k,$$

and the transformation $E_n(C_m)$ is actually operating with the following terms. From the practical point of view, this has the advantage that, by selecting appropriate values for m, one can concentrate on using the transformation technique over the terms of the series for which some kind of monotonous or asymptotic behavior is present. In this way, allowance is made for faster converging resulting sequences.

3. SUMMATION OF PARTIAL WAVE EXPANSIONS

In atomic and molecular collision processes the interactions are frequently represented by central potentials with a long-range behavior

$$V(r)\sim\frac{A}{r^{\alpha+2}},\quad \alpha\geqslant -1, \tag{3.1}$$

where α is an integer and A a constant. Depending on the particular process and of the energy involved, this determines that even very high angular momentum partial waves will give an important contribution in the expansion of the scattering amplitude

$$f(\theta)=\frac{1}{2ik}\sum_{L=0}^{\infty}(2L+1)\ [\exp(2i\delta_L)-1]P_L(\cos\theta), \tag{3.2}$$

as well as in that of the total elastic cross section

$$Q=\frac{4\pi}{k^2}\sum_{L=0}^{\infty}(2L+1)\ \sin^2\delta_L, \tag{3.3}$$

where k is the magnitude of the wave vector, the δ_L are the phase shifts, and the P_L are the Legendre polynomials. Because of this fact, the expansions in Eqs. (3.2) and (3.3) are slowly convergent, and in certain physical problems it is necessary to deal with thousands of phase shifts.[9] For these cases, the exact computation of all the δ_L is prohibitive, and different approximations are used for the high order ones.[10] However, the numerical work can still be considerable. An example is the empirical determination of an interaction potential. A usual method,[11] is to start with a potential given by an analytical expression dependent on parameters, to which approximate values are given. Then the δ_L are calculated and a comparison is set between the theoretical and experimental cross sections. Repeating the procedure for different values of the parameters, they are determined by "trial and error," by seeking an accurate fit. Since each step requires the determination of the corresponding phase shifts, it is clear that the numerical efforts will be very important when many partial waves are necessary in the calculations.

In this work, the methods of Sec. 2 are applied for the summation of expansion (3.2). In a precedent paper,[1] the formal asymptotic convergence properties of the PPA were

studied when dealing with this type of application. It was shown that for a potential with a long-range tail, as that given by Eq. (3.1), the PPA $[n,n+m]$ to the expansions of $f(\theta)$ and Q, have, for fixed n and $m\to\infty$, the following asymptotic behaviors.

$$[n,n+m]_{f(0)}\sim f(0)+\frac{K(\alpha-2)!n!}{(n+\alpha-1)!M^{\alpha-1}},\quad (\alpha\geqslant 2), \tag{3.4a}$$

$$[n,n+m]_{f(\theta)}\sim f(\theta)+\frac{(-1)^{N+1}K(\sin\theta)^{2(n-N)-1/2}2^{N-2n}(2\alpha+2N-1)!!N!\,(\sin\Lambda_{m+n})^{2(2N-n)+1}}{(2\pi)^{1/2}(2\alpha-1)!!(\sin\theta/2)^{2n+1}M^{\alpha+2N+1/2}} \tag{3.4b}$$

$(\alpha\geqslant 0,\ 0<\theta<\pi,\ \sin\Lambda_{m+n}\neq 0,$

$[n,n+m]_{f(\pi)}\sim f(\pi)$

$$+\frac{(-1)^{m+1}K(\alpha+n-1)!n!}{2^{2n+1}(\alpha-1)!M^{\alpha+2n}}\quad (\alpha\geqslant 1), \tag{3.4c}$$

$$[n,n+m]_{Q}\sim Q+\frac{K'}{2\alpha}\frac{(2\alpha)!n!}{(n+2\alpha)!M^{2\alpha}}\quad (\alpha\geqslant 1), \tag{3.4d}$$

where $K=Ak^{\alpha-1}I_\alpha$, $\Lambda_j=(j+1)\theta-\pi/4$, $M=m+1/2$; $N=n/2$ for even n, $N=(n-1)/2$ for odd n, $K'=2\pi A^2k^{2\alpha-2}I_\alpha^2$, and

$$I_\alpha=\begin{cases}\dfrac{\pi}{2} & \text{for } \alpha=0\\[2ex] \dfrac{(\alpha-1)!!}{\alpha!!}\dfrac{\pi}{2} & \text{for even } \alpha>0,\\[2ex] \dfrac{(\alpha-1)!!}{\alpha!!} & \text{for odd } \alpha\end{cases}$$

The conditions imposed on α in Eqs. (3.4) are the usual ones to assure that expansions (3.2) and (3.3) are convergent. A comparison can be set between the asymptotic rates of convergence given by Eqs. (3.4a)–(3.4c) for $n>0$, with that of the sequences of partial sums of the corresponding expansions, i.e., the $[0,m]_{f(\theta)}$. It is seen that when going to the nth row of the Padé table ($n>0$), the rate of convergence is increased, relative to the first ($n=0$), by factors of the order of $(\alpha-1)n!/(n+\alpha-1)!$ ($\theta=0$, $\alpha\geqslant 2$), $(1/m)^n$ ($0<\theta<\pi$, $\alpha\geqslant 0$), and $(1/m)^{2n}$ ($\theta=\pi$, $\alpha\geqslant 1$). Furthermore, the behavior of the $[n,n+m]_Q$ is essentially similar to that of $[n,n+m]_{f(0)}$ [cf. Eqs. (3.4a) and (3.4d)].

The discussion above concerns asymptotic properties, and motivates the use of PPA. In the next section, their practial significance is investigated.

4. NUMERICAL APPLICATIONS TO PHYSICAL PROBLEMS

In this section, the numerical application of the transformation procedures outlined in the preceding ones is considered for the summation of slowly convergent, divergent and oscillating partial wave expansions of the scattering amplitude. Four cases are studied. They are representatives in the field of atomic and molecular processes, of those in which the calculation of the scattering amplitude from the partial wave expansion is troublesome. They are:

(A) The elastic e–He collision in the range 100–400 eV;

(B) The scattering by a Lennard–Jones potential;

(C) The scattering by a repulsive inverse square potential;

(D) Coulomb scattering.

For these cases, the rows of the Padé table, i.e., the approximants $[n,n+m]$ with fixed n, were calculated by means of the η algorithm. Other sequences of the table could be considered. One of these could be the usual near diagonal PPA $[n,n+m]$ with fixed m. However, the numerical work involved in calculating a $[n,n+m]$ from the partial sums, by using the η algorithm, increases as n^2. This suggests keeping n as low as possible, although, the numerical evidence indicates that the accuracy of the PPA increases with n, as predicted by the asymptotic estimates [cf. Eqs. (3.4a)–(3.4c)].

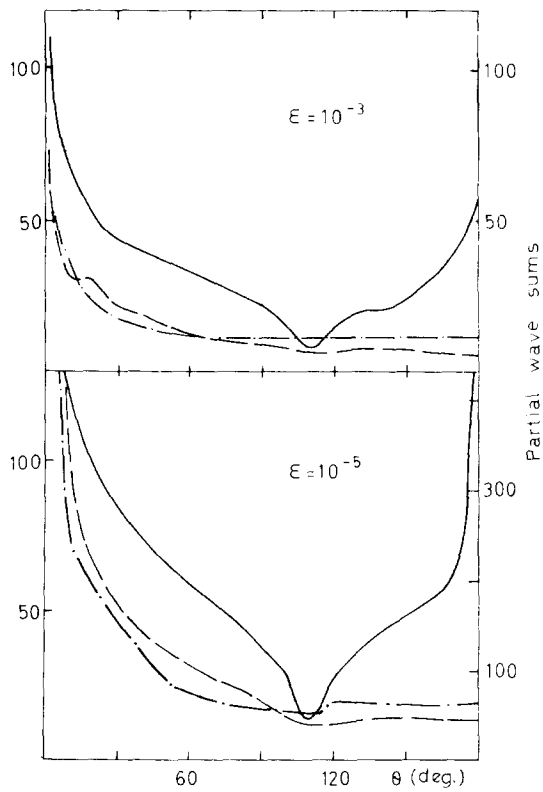

FIG. 1. Case (A) elastic e-He scattering. Number of partial waves required to obtain the elastic differential cross section within an accuracy ϵ, by using different PPA; solid line: partial wave sums ($[0,0+m]$); dashed line: $[2,2+m]$; dash-dotted line: $[5,5+m]$. The scale on the right corresponds to the partial wave sums.

TABLE I. Electron–helium scattering at 100 eV. Number of partial waves required to obtain, by using PPA, the forward cross section with the indicated accuracies.

ϵ	$[0,0+m]$	$[1,1+m]$	$[2,2+m]$	$[3,3+m]$
10^{-2}	300	160	110	80
10^{-3}	3000	1580	1040	780

Here, the main interest is to compare the efficiency of different PPA when calculating the differential cross section. The efficiency measure of an approximation has been taken as the number of partial waves required to obtain a given accuracy. It is assumed that a sequence A_m is approximating the value A within an accuracy ϵ, by using m_0 partial waves, if m_0 is the least integer such that $|A_m - A|/|A| < \epsilon$ for $m > m_0$. The method used for the determination of the reference "exact" value A, will be indicated for each particular interaction.

A. Elastic electron–Helium collision

The phase shifts given by the extended polarization method studied by La Bahn and Callaway[9] have been used for energies in the range 100–400 eV. The asymptotic behavior of the interactions involved is of the electron-induced dipole type [$V(r) \underset{r\to\infty}{\sim} A/r^4$]. Then, the asymptotic theorems [Eqs. (3.4)] are valid in this case.

The reference values were calculated with higher order $[n,n+m]$ PPA, n ranging from 10 to 200. In this way, it was possible to obtain $|f(\theta)|^2$ with four and eight significant figures for $\theta=0$ and $\theta\neq 0$, respectively.

In Fig. 1, the number of partial waves required to attain accuracies $\epsilon = 10^{-3}$ and 10^{-5}, with the low order PPA $[2,2+m]$ and $[5,5+m]$, is plotted as a function of the scattering angle, for the energy $E = 100$ eV. A comparison is set with the corresponding curves for the partial wave sums. Results for the critical case $\theta = 0$ are shown in Table I. Similar behaviors are obtained for the other energies.

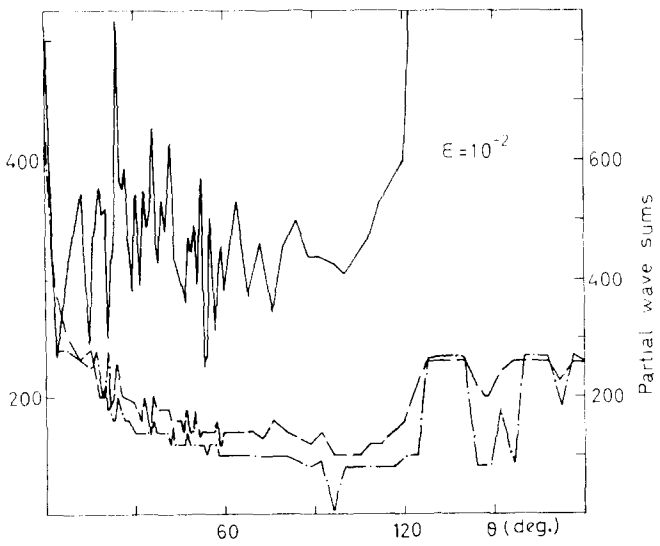

FIG. 2. Case (B) scattering by a Lennard–Jones potential. Captions as in Fig. 1, $\epsilon = 10^{-2}$.

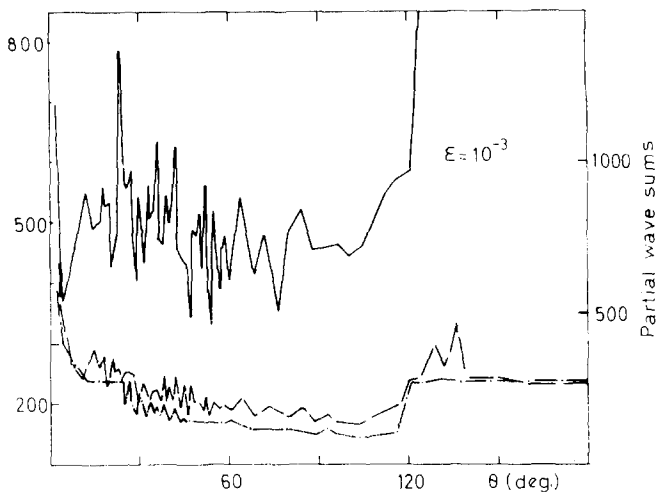

FIG. 3. Same as in Fig. 2, $\epsilon = 10^{-3}$.

B. Scattering by a Lennard–Jones potential

The scattering of particles with a reduced mass μ by a (6,12) L–J potential

$$V(r) = 4V_0\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

can be parametrized by means of the de Boer parameter $\Omega = h/(2\mu V_0\sigma^2)^{1/2}$ and the reduced energy $e = E/V_0$. The calculation was performed in the range $\Omega < 0.3$, where rainbow scattering occurs[12] and where the covergence of the partial wave expansion is worst. In this range, the phase shifts are well represented by the semiclassical JWKB approximation,[13] and were calculated by using a Gauss–Mehler quadrature, as proposed in Ref. 12.

The reference values were determined as in the precedent application. In Figs. 2 and 3 the case $\Omega = 0.1$, $e = 2$ is studied for relative accuracies $\epsilon = 10^{-2}$ and 10^{-3}, respectively. Similar results can be found for other values of the parameters, in the Ω range considered. For fixed θ, the number of partial waves increases considerably when Ω decreases and (or) e increases.

By inspection of the figures, it can be seen that the relative error of the partial sums is a strongly oscillating function of θ. This behavior is closely related to the interference effects which, in turn, are responsible for the high frequency quantum oscillations of the scattering amplitude, typical for this kind of potentials. The relative error curves for the PPA show a considerable attenuation of the oscillations, which increases with n. The plots have been made with a 0.5 degree step in the rainbow scattering range (15°–60°)[12] and a four degree one elsewhere. Further oscillations between the suc-

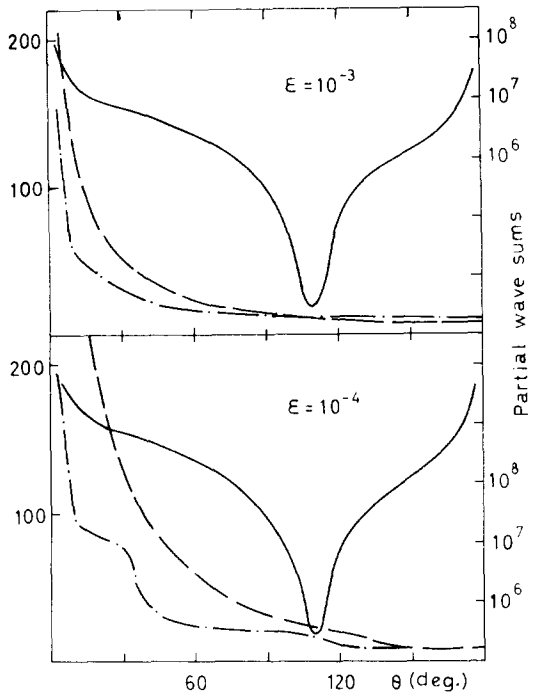

FIG. 4. Case (C) scattering by a repulsive inverse square potential. Captions as in Fig. 1. The number of partial waves involved in the calculations with the partial sums, have been determined by recurrent use of Eq. (3.4b).

cessive angles considered do not modify the comparative analysis of the approximations.

C. Scattering by a repulsive inverse square potential

For the potential $V(r)=g/r^2$ $(g>-\frac{1}{4})$ the exact phase shifts are energy independent, and are given by

$$\delta_L=\frac{\pi}{2}\{L+\tfrac{1}{2}-[(L+\tfrac{1}{2})^2+g]^{1/2}\}.$$

The reference values of $f(\theta)$ can be obtained with any required accuracy by a method described in a previous paper.[14] The case $g=1$ is considered. The general qualitative features of the results do not change by increasing g. In Fig. 4 significant curves are shown for this potential. For $\theta=0$ the exact $f(\theta)$ has a branch point, no rational approximation can be accurate, and the partial wave expansion diverges. This explains the unbounded increase of the relative error curves of the PPA as $\theta\to 0$. For $\theta=\pi$ the partial wave sums for $f(\theta)$ are oscillatory and do not define $f(\pi)$,[14] then, their error curves go to infinity as $\theta\to\pi$. The PPA give finite and accurate values for $f(\pi)$, illustrating their power as a regularizing mechanism.

D. Coulomb scattering

The scattering amplitude for the potential

$$V(r)=2\beta/r$$

can be characterized by the parameter $\gamma=\beta/k$, where k is the magnitude of the wave vector. This is a very interesting case because the PPA approach proves again to be a powerful regularizing method. The amplitude $f(\theta)$ is well defined, for $\theta\neq 0$, by

$$f(\theta)=\frac{-\gamma^2}{1-\cos\theta}\exp\{2i\sigma_0-i\gamma\ln[(1-\cos\theta)/2]\}.$$

However, the expansion

$$f(\theta)\doteq\frac{|\mathcal{M}|}{2i}\sum_{L=0}^{\infty}(2L+1)\exp(2i\sigma_L)P_L(\cos\theta),$$

where $\sigma_L=\arg\Gamma(L+1+i\gamma)$, is divergent, and is only a formal representation of the amplitude.

In Fig. 5 representative results are shown for $\gamma=1$. Again, changes in the value of γ preserve the general qualitative behavior of the approximations, and only affect the number of partial waves involved for each θ. The convergence of the PPA is fast over all the angular range, except for $\theta\to 0$. For $\cos\theta=1$ the $f(\theta)$ has a branch point and the rational approximation scheme fails, as in the preceding application.

5. DISCUSSION

In Sec. 4 it has been shown, that the number of phase shifts required to obtain the differential cross section with a prescribed accuracy, can be remarkably reduced when the PPA approach is used as an alternative summation method to that of the partial wave sums. We have not found fixed rules allowing one to select the most efficient PPA for a given application, although some hints can be obtained from the numerical results. In general, it can be seen that, as shown by Figs. 1–5, the error curves corresponding to PPA with different orders n, tend to overlap as the accuracy requirements decrease. This fact suggests that low order transformations

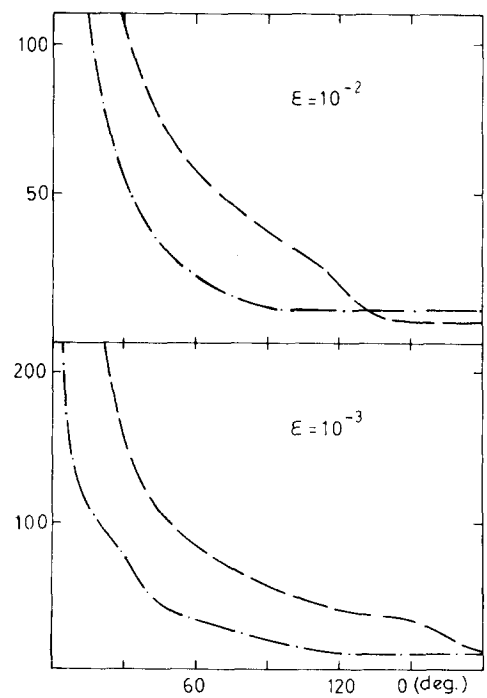

FIG. 5. Case (D) Coulomb scattering. Captions as in Fig. 1.

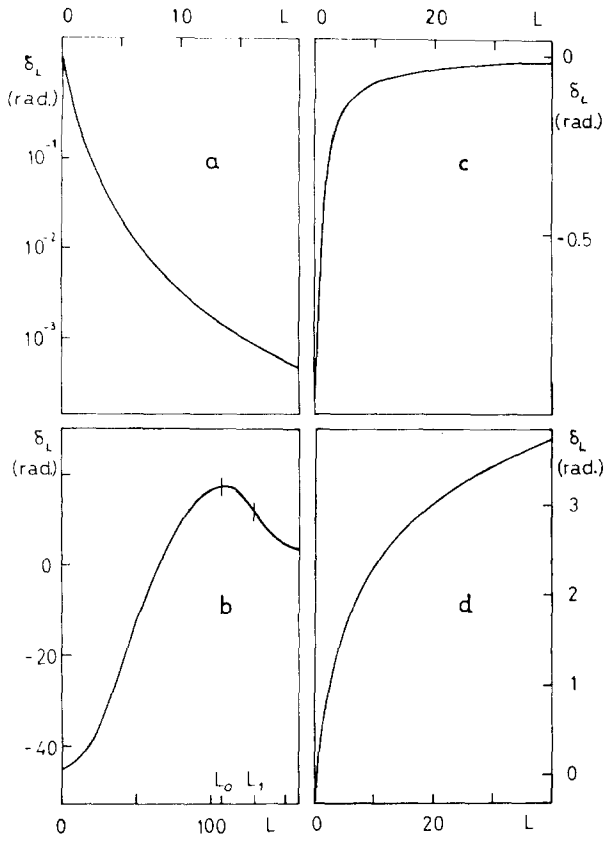

FIG. 6. Phase shifts δ_L as functions of angular momentum L for the cases considered.

should be preferred when relatively low accuracies are sought.

As noted by the end of Sec. 2, the calculation of the $[n,n+m]$ PPA is equivalent to starting to transform the original series from its mth term, and it can be of advantage to have criteria for selecting a proper least value for m. In order to discuss this possibility, for the applications here considered, the corresponding phase shifts δ_L have been plotted in Fig. 6, as functions of L. For cases (A), (C), and (D), where monotonous δ_L are involved, no special least value for m has been found. In principle, the PPA transformations can begin from the first term of the partial wave expansion, although keeping n as low as possible. For the Lennard–Jones potential [case (B)], the PPA give convergent results, when the number of phase shifts employed in the calculations is greater than L_1, the inflection point of the function $\delta_L = \delta(L)$. By adding up the first L_1 partial waves of the expansion, and transforming the series from there on, the convergence of the PPA is fast, particularly in the rainbow scattering region. It is to be noted that the information used in this way is similar to that required by the semiclassical approximation methods.[15]

Numerical convergence is attained quite before the δ_L reach their asymptotic Massey–Mohr expression.[1] This fact shows that one of the conditions used to obtain Eqs. (3.4) is not actually necessary to assure the convergence of the PPA. This stresses the importance of the approach from the practical point of view.

Regarding the behavior of the error curves as a function of the scattering angle θ, the results agree, qualitatively, with the asymptotic predictions of Eqs. (3.4a)–(3.4c), when these apply. The relative error displayed in the figures is essentially given by

$$\epsilon \simeq 2 \frac{|\mathrm{Re} f(\theta)|}{|f(\theta)|^2} \left| \mathrm{Re} f(\theta) - \mathrm{Re}[n,n+m]_{f(\theta)} \right|, \tag{5.1}$$

since the contribution of the error of $\mathrm{Im}[n,n+m]_{f(\theta)}$ is negligible compared to that of $\mathrm{Re}[n,n+m]_{f(\theta)}$. To simplify the discussion, consider $\theta \neq 0$, and n even. Then, using Eq. (3.4b) in (5.1),

$$\epsilon \simeq 2 \frac{|\mathrm{Re} f(\theta)| \ (\sin\theta)^{n-1/2} (2\alpha+n-1)!! \sin\Lambda_{m+n}}{|f(\theta)|^2 (\sin\theta/2)^{2n+1} (2\pi)^{1/2} (2\alpha-1)!! m^{\alpha+n+1/2}} \tag{5.2}$$

with $\alpha \geqslant 0$. When $n=0$, i.e., for the partial wave sum, the factor $[\sin^2(\theta/2)\sin\theta]^{-1/2}$ predicts an increase of ϵ for $\cos\theta \to \pm 1$, and a minimum at $\theta_m = 120°$. The curves corresponding to cases (A) and (C) show these general features. A slight shift in the position of the minimum can be easily seen to be due to the factor $R(\theta) = |\mathrm{Re} f(\theta)|/|f(\theta)|^2$. In case (B), $R(\theta)$ is also responsible for the fast increase of the curves for $\theta \geqslant \theta_m$. This fact can be traced down to a strong cancellation between the contributions to the scattering amplitude coming from the partial waves for $L < L_0$ and those with $L > L_0$. Furthermore, the strong oscillations of $R(\theta)$ disguise the expected minimum of the curves.

For $n \neq 0$ in Eq. (5.2), the factor $(\sin\theta)^{n-1/2} \cdot (\sin^2\theta/2)^{-n-1/2}$ decreases monotonously with increasing θ, consistently with the results obtained for cases A and C. This is expected on physical grounds, i.e., as θ increases the contribution of the waves with large angular momentum should become less important. For the Lennard–Jones potential, the slight increase at $\theta \sim \theta_m$ followed by an essentially flat behavior, can be explained as due to the factor $R(\theta)$ and the indefinite sign potential.

A remark should be made regarding the importance of the PPA approach as a regularizing procedure for divergent and oscillatory partial wave expansions, as seen in applications (D) and (C) (for $\theta = \pi$), respectively. Many of the general features discussed above also apply to these cases. This suggests that the convergence domain of the PPA is actually larger than that given by the convergence theorems.[16] Moreover, the PPA may be well behaved even for values of $\cos\theta$ outside the physical interval $[-1,1]$, and hence be a powerful method for the analytical continuation of the scattering amplitude into the complex $\cos\theta$ plane.

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On the matrix representation of closed linear operators: An extension of the Von Neumann's theory

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The general theory of the matrix representation of operators in scalar product space is examined. It is proved that an extension of the Von Neumann's theory on the matrix representation of closed symmetric operators in Hilbert space is possible for a larger class of closed operators. A necessary and sufficient condition for the existence of a matrix representation of operators in "Von Neumann's sense" is given.

1. INTRODUCTION

The problem of the matrix representation of an operator A with domain D_A in a separable scalar product space D consists essentially of two parts:

(a) To find, for a fixed orthonormal basis (e_ν) in D, a matrix $(A_{\mu\nu})$ which allows to determine for any vector $\varphi=\Sigma_{\nu=1}^{\infty}\xi_\nu e_\nu\in D_A$ its image $\psi=A\varphi$, i.e., the components η_μ of the vector ψ.

(b) To determine the exact relation between the operator A and the matrix $(A_{\mu\nu})$, so that it is possible to obtain the operator A from the matrix $(A_{\mu\nu})$ and the basis (e_ν).

The part (a) has been solved, relatively to any orthonormal basis chosen in the space, for the operator[1] of $B(H)$ and for those[2] of C_D by means of the generalizated closure equation or using the weak[3] continuity of the operators.

The part (a) of the problem is also solved for any operator A, defined in a separable scalar product space D, which admits an adjoint A^* with $\overline{D_A\cap D_{A^*}}=D$, relatively to any basis chosen in $D_A\cap D_{A^*}$ by means of the generalizated closure equation.[4]

We prove in this paper that in the last case part (a) can be solved using the continuity of the operator A in some suitable weak topologies that is equivalent to the existence of the adjoint operator.

The matrix $(A_{\mu\nu})$ in all cases is determined by the relations

$$A_{\mu\nu}=(Ae_\nu,e_\mu),\quad \mu,\nu=1,2,\cdots.$$

Problem (b) is more complicated. The complication consists in the fact that, even if it is possible to construct a matrix $(A_{\mu\nu})$, in the sense of problem (a), the domain of this matrix is different from that of the operator A because the set

$$D_{(A_{\mu\nu})}=\left\{\varphi=\sum_{\nu=1}^{\infty}\xi_\nu e_\nu\in D:\sum_{\mu=1}^{\infty}\left|\sum_{\nu=1}^{\infty}A_{\mu\nu}\xi_\nu\right|^2<\infty\right\}$$

is generally larger[5] than D_A. Hence A and $(A_{\mu\nu})$ are different operators and there is no general connection between these operators.

It is obvious that these pathologies do not arise if the domain of the operators is the whole space, as it happens for the operators of $B(H)$ and for those of C_D.

Hence it is clear that if it is easy to give a definition for the matrix representation of the operators of $B(H)$ or C_D, it is not equally easy for other operators.

These difficulties have been overcome by von Neumann,[6] for the closed symmetric operators in Hilbert space H, introducing a suitable definition of matrix representation. He observed that if A is a closed symmetric operator, densely defined in a separable Hilbert space H, and (e_ν) any orthonormal basis in D_A, letting $A_{\mu\nu}=(Ae_\nu, e_\mu)$, the closure of the operator R defined by the matrix[7] on the linear envelope $\{e_\nu\}^L$ is generally a restriction of A, i.e., $\overline{R}\subseteq A$. Von Neumann proved that there exists an orthonormal basis in D_A for which $\overline{R}=A$. In this case von Neumann said that the matrix $(A_{\mu\nu})$ "represents" the operator A relatively to the basis (e_ν).

We have proved in this paper that the von Neumann's theory can be extended to a larger class of closed operators in a separable Hilbert space H. This class, obviously, includes, the closed symmetric operators.

We have also given a necessary and sufficient condition in order that a closed operator in H admit a matrix representation in von Neumann's sense.

2. MATRIX REPRESENTATION OF UNBOUNDED OPERATORS IN SCALAR PRODUCT SPACE

Definition 1: Let E, F be two linear manifolds of a scalar product space D. We say that E is endowed of the F-weak topology[8] if the topology in E is determined by the set of seminorms

$$\{\varphi\to|(\varphi,\psi)|/\varphi\in E\}_{\psi\in F}.$$

If both E and F are dense in D the topology is a Hausdorff one.

Theorem 1: Let E, F be two dense linear manifolds of D and A an operator with domain $D_A=E$; the following propositions are equivalent[9]:

(i) A is continuous for the topologies $\sigma(E,D)\to\sigma(D,F)$

(ii) There exists the operator A^* (adjoint of A) with domain $D_{A^*}\supseteq F$.

It is obvious that $\sigma(D,D_{A^*})$ is the strongest of the σ-topologies in D for which A is continuous. It is also obvious that A^* is continuous in the topologies $\sigma(D_A,D)\to\sigma(D,D_{A^{**}})$.

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From now on, we assume that the scalar product spaces that we consider are separable.

Theorem 2: Let A be a linear operator in a scalar product space D, with domain D_A, which admits an adjoint A^* such that $\Delta = D_A \cap D_{A^*}$ is dense in D, let (e_ν) be an orthonormal basis in D for which $e_\nu \in \Delta$, $(\nu = 1,2,\cdots)$. Letting $A_{\mu\nu} = (Ae_\nu, e_\mu)$ for $\varphi = \Sigma_{\nu=1}^{\infty} \xi_\nu e_\nu \in D_A$ and $\psi = A\varphi = \Sigma_{\nu=1}^{\infty} \eta_\nu e_\nu$, we have

$$\eta_\mu = \sum_{\nu=1}^{\infty} A_{\mu\nu} \xi_\nu .$$

Proof[10]: Since we consider here both the norm topology defined by the scalar product and the weak topology of Definition 1, we use in this proof the symbols "s" (strong) and "w" (weak) to indicate the limits in the first and second topology respectively.

Let (e_ν) be the fixed orthonormal basis, since the restriction of the norm topology in D_A is stronger than $\sigma(D_A, D)$ we have

$$\forall\ \varphi \in D_A$$

$$\varphi = \sum_{\nu=1}^{\infty} \xi_\nu e_\nu = \lim_{n\to\infty}{}^{s} \sum_{\nu=1}^{n} \xi_\nu e_\nu$$

$$= \lim_{n\to\infty}{}^{w} \sum_{\nu=1}^{n} \xi_\nu e_\nu$$

$$\text{Then} \forall\ \varphi \in D_A \quad (A\varphi)_\mu = (A\varphi, e_\mu)$$

$$= \left(A \lim_{n\to\infty}{}^{w} \sum_{\nu=1}^{n} \xi_\nu e_\nu, e_\mu \right)$$

$$= \lim_{n\to\infty} \sum_{\nu=1}^{n} \xi_\nu (Ae_\nu, e_\mu)$$

$$= \sum_{\nu=1}^{\infty} \xi_\nu A_{\mu\nu} .$$

We have made use here of the linearity of A and of its continuity in the topologies $\sigma(D_A, D) \to \sigma(D, D_{A^*})$.

Since A^* (which also has dense domain) is continuous in the topologies $\sigma(D_{A^*}, D) \to \sigma(D, D_{A^{**}})$ we can, in an analogous way, prove that

$$(A^*\varphi)_\mu = \sum_{\nu=1}^{\infty} \xi_\nu A^*_{\mu\nu} = \sum_{\nu=1}^{\infty} \xi_\nu \overline{A}_{\nu\mu}$$

$$\forall \varphi = \sum_{\nu=1}^{\infty} \xi_\nu e_\nu \in D_{A^*} .$$

The matrices obtained by the operators A and A^* are the adjoints of each other and satisfy the relations:

$$\sum_{\mu=1}^{\infty} \left| \sum_{\nu=1}^{\infty} A_{\mu\nu} \right|^2 < \infty, \quad \sum_{\nu=1}^{\infty} \left| \sum_{\mu=1}^{\infty} A_{\mu\nu} \right|^2 < \infty .$$

Notice that only with an operator which satisfies the conditions of Theorem 2 can we associate a matrix in the sense of point (a) of the Introduction, because the proof of this theorem emphasizes that the basis must belong to $D_A \cap D_{A^*}$ and the operator must be continuous in the sense of Theorem 1.

We will now consider point (b) of the Introduction. This problem is solvable only for some closed operators defined in complete scalar product space (Hilbert space).

Definition 2: Let $(A_{\mu\nu})$ be a squarable matrix, i.e., a matrix for which

$$\sum_{\nu=1}^{\infty} |A_{\mu\nu}|^2 < \infty \quad \text{and} \quad \sum_{\mu=1}^{\infty} |A_{\mu\nu}|^2 < \infty .$$

Let (e_ν) be an orthonormal basis in H and R the operator defined by the matrix $(A_{\mu\nu})$ on the basis vectors letting

$$Re_\nu = \sum_{\mu=1}^{\infty} A_{\mu\nu} e_\mu$$

and extending by linearity to the linear envelope $\{e_\nu\}^L$ of (e_ν), and $\overline{R}$ its closure. We say that $\overline{R}$ is the operator yielded by the pair matrix basis $\{(A_{\mu\nu}), (e_\nu)\}$.

In an analogous way, we can introduce the operator $\overline{R'}$ yielded by the pair matrix basis $\{(A^*_{\mu\nu}), (e_\nu)\}$. Generally the operator $\overline{R'}$ is not the adjoint of the operator $\overline{R}$.

Definition 3: Let A be a closed densely defined operator in H which admits an adjoint A^* such that $\Delta = D_A \cap D_{A^*}$ is dense in H. We say that the basis (e_ν) is a basis for a matrix representation of the operator A if:

(i) the elements of the basis belong to Δ,

(ii) letting $A_{\mu\nu} = (Ae_\nu, e_\mu)$, the operator $\overline{R}$, yielded by the pair matrix basis $\{(A_{\mu\nu}), (e_\nu)\}$, coincides with A.

Theorem 3: Let A be a closed operator in H which admits an adjoint A^* such that $\Delta = D_A \cap D_{A^*}$ is dense in H, and (e_ν) a basis in Δ; the following two propositions are equivalent:

(i) $\forall\ \varphi \in D_A$ there exists a sequence $\{\varphi_n\} \subseteq \{e_\nu\}^L$ such that $\varphi_n \to \varphi$ and $A\varphi_n \to A\varphi$.

(ii) The basis (e_ν) is a basis for a matrix representation of the operator A.

Proof: We prove first that (i)$\Rightarrow$(ii).

Letting $A_{\mu\nu} = (Ae_\nu, e_\mu)$ and $A^*_{\mu\nu} = \overline{(Ae_\mu, e_\nu)}$, we can define the operator T' by the relation

$$T'\psi = \sum_{\nu=1}^{\infty} \eta_\nu e_\nu$$

with

$$\eta_\mu = \sum_{\nu=1}^{\infty} \overline{A}_{\nu\mu} \xi_\nu$$

on the set $D_{T'}$ of all vectors $\psi = \Sigma_{\nu=1}^{\infty} \xi_\nu e_\nu$ for which

$$\sum_{\mu=1}^{\infty} \left| \sum_{\nu=1}^{\infty} \overline{A}_{\nu\mu} \xi_\nu \right|^2 < \infty$$

we prove that $A^* = T'$.

In fact, it is obvious that $A^* \subseteq T'$. We show now that $T' \subseteq A^*$.

Let $\psi \in D_{T'}$, with $\psi = \Sigma_{\nu=1}^{\infty} \xi_\nu e_\nu$, we have

$$(Ae_\mu,\ \psi)=\sum_{\nu=1}^{\infty}\bar{\xi}_\nu(Ae_\mu,\ e_\nu)=\sum_{\nu=1}^{\infty}A_{\nu\mu}\bar{\xi}_\nu.$$

On the other hand we have

$$(T'\psi,e_\mu)=\sum_{\nu=1}^{\infty}\bar{A}_{\nu\mu}\xi_\nu.$$

Hence we obtain

$$(Ae_\mu,\ \psi)=\overline{(T'\psi,e_\mu)}=(e_\mu,\ T'\psi)$$

by linearity, it follows that

$$(Af,\psi)=(f,T'\psi)\quad\forall f\in\{e_\nu\}^L,\quad\psi\in D_{T'}.$$

If $\varphi\in D_A$, by the hypothesis, there exists a sequence $\{\varphi_n\}\subseteq\{e_\nu\}^L$ such that $\varphi_n\to\varphi$ and $A\varphi_n\to A\varphi$; then we have

$$(A\varphi,\psi)=(\lim_{n\to\infty}A\varphi_n,\psi)=\lim_{n\to\infty}(A\varphi_n,\psi)$$

$$=\lim_{n\to\infty}(\varphi_n,T'\psi)=(\lim_{n\to\infty}\varphi_n,T'\psi)$$

$$=(\varphi,T'\psi).$$

Hence $\psi\in D_{A^*}$ and $A^*\psi=T'\psi$, i.e., $T'\subseteq A^*$.

In order to complete this part of the proof, we consider the operator R. It is obvious that R^* exists and $R^*\subseteq T'$; we have then

$$R^*\supseteq A^*=T',\qquad R^*\subseteq T'=A^*,$$

i.e., $R^*=A^*$ and, since the space H is complete, $\bar{R}=A$.

Conversely, suppose that (ii) is satisfied. The operator $\bar{R}$ is defined, as it is known, from R adding to $D_R=\{e_\nu\}^L$ all those elements of $\bar{D}_R$ which are limits of sequences $\{f_n\}\subseteq D_R$ generating convergent sequences Rf_n and requiring that $\bar{R}f=\lim_{n\to\infty}Rf_n$; i.e., (ii)$\Rightarrow$(i).

We shall now prove that the matrix representation is possible only for a special class of closed operators.

Definition 4: Let A be a closed operator which admits an adjoint A^* such that $\Delta=D_A\cap D_{A^*}$ is dense in H. We say that A is a Δ-minimal operator if for every closed operator B such that

$$A\supseteq B\supseteq A/\Delta$$

we have $A=B$.

Theorem 4: Let A be a closed operator which admits an adjoint A^* such that $\Delta=D_A\cap D_{A^*}$ is dense in H. In order that there exist a basis for a matrix representation of the operator A, it is necessary and sufficient that A be a Δ-minimal operator.

Proof: We prove first necessity. We suppose that there exists a basis (e_ν) for a matrix representation of A. Let B be a closed operator for which

$$A\supseteq B\supseteq A/\Delta.$$

By definition, $\bar{R}=A$. But, on the other hand, B is a closed operator and $R\subseteq B$, hence $\bar{R}\subseteq B$, so that $B=A$, i.e., A is a Δ-minimal operator.

Now we prove the sufficience. In $H\oplus H$ we consider the graph of the operator A, that is, the set

$$G_A=\{\{\varphi,A\varphi\}/\varphi\in D_A\}.$$

It is known that G_A is a subspace of $H\oplus H$. We consider now the graph of A/Δ, which we call G',

$$G'=\{\{\varphi,A\varphi\}/\varphi\in\Delta\}.$$

It is obvious that G' is a linear manifold of G_A. We prove that, in our hypothesis, G' is dense in G_A. In fact, if G' is not dense in G_A, we have $\overline{G'}\subset G_A$, so that $\overline{G'}$ is the graph of a closed operator B and $D_B\supseteq\Delta$. Hence

$$A\supset B\supseteq A/\Delta$$

and so A is not a Δ-minimal operator, in contrast with the hypothesis. We conclude that G' must be dense in G_A.

Then in G' it is possible to find a basis for G_A. We call it $(\{f_\mu,\ Af_\mu\})$; consequently, $\{f_\mu\}$ is dense in Δ and hence in H. In order to obtain a basis satisfying the condition (ii) of Theorem 3 it remains only to orthogonalize the sequence $\{f_\mu\}$.

It is evident that a closed symmetric operator A with dense domain D_A is a D_A-minimal operator; hence the von Neumann's theory is a particular case of this theorem.

Definition 5: Let A be a closed operator which admits an adjoint A^* such that $\Delta=D_A\cap D_{A^*}$ is dense in D. We say that A is a Δ-maximal operator if for every closed operator B such that

$$A^*\supseteq B^*\supseteq A^*/\Delta$$

$A=B$ results.

We say that the operator A is Δ-simple if it is both Δ-minimal and Δ-maximal.

It follows from the Definitions 4 and 5 that the operator A is Δ-maximal iff its adjoint is Δ-minimal and that a closed operator is Δ-simple iff its adjoint is also Δ-simple.

It is easy to prove, using Theorem 4 and Definition 5, the following:

Theorem 5: Let A be a closed operator, which admits an adjoint A^*, such that $\Delta=D_A\cap D_{A^*}$ is dense in H. In order that there exist a basis (e_ν) for a matrix representation of A and a basis for a matrix representation of A^*, it is necessary and suffficient that A be a Δ-simple operator.

The last theorem does not imply that if A and A^* admit a matrix representation in the sense of Definition 2, the basis for this representation is the same for both. This appears clear from the following:

Theorem 6: Let (e_ν) be a basis for a matrix representation of the Δ-simple operator A. The basis (e_ν) is also a basis for a matrix representation of the operator A^* if, and only if, one has

$$T'=T^*,$$

where the operator T' is what we have defined in the proof of Theorem 3 and the operator T is defined in an analogous way,[11] exchanging the matrix $(A^*_{\mu\nu})$ with the matrix $(A_{\mu\nu})$.

Proof: If (e_ν) is a basis for a matrix representation of both A and A^* we have, by Theorem 3

$$A^*=T' \quad \text{and} \quad A=T$$

and since T', T, A, A^* are closed it follows that

$$T^*=A^*=T'.$$

If $T'=T^*$, since A admits a matrix representation with respect to the basis (e_ν), it follows, by Definition 2 and Theorem 3, that $T'=A^*$, hence $T^*=A^*$; i.e., $T=A$. Now, if we call R' the operator defined by the matrix $(A^*_{\mu\nu})$ on the linear envelope $\{e_\nu\}^L$, $\overline{R'} \subseteq A^*$. But, since, as one sees immediately, $(R')^* \subseteq T$, it follows that

$$(R')^{**} \supseteq T^* = A^*, \quad \text{i.e.,} \quad \overline{R'} \supseteq A^*..$$

Hence $\overline{R'}=A^*$ and, by Definition 2, the matrix $(A^*_{\mu\nu})$ represents the operator A^* with respect to the same basis (e_ν).

Since, generally, a closed symmetric operator A is not Δ-simple, there does not exists a basis for a representation of A^*. In fact a closed symmetric operator is Δ-simple iff it is self-adjoint; in this case it follows easily by the last theorem that

$$T'=T.$$

It is obvious that the matrix representation of a Δ-minimal operator A $(\Delta=D_A \cap D_{A^*})$ leads, generally, both for the operations and for the change of basis, to the same pathologies that von Neumann pointed out for the closed symmetric operators. Hence these pathologies make the use of matrices unsuitable for the study of unbounded operators. Notice that the use of the matrix representation does not present difficulties if they belong to C_D

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APPENDIX

Let us give a proposition which supplies a practical way to construct a Δ-simple operator which is, generally, neither bounded nor self-adjoint.[12]

Theorem 7: Let $M_1, M_2, \ldots, M_i \cdots$ be a sequence of subspaces of a Hilbert space H which are mutually orthogonal and such that

$$H \simeq \bigoplus_{i=1}^{\infty} M_i.$$

If $f \in H$, we call f_i its projection of M_i.

Let A_i be a given linear bounded operator invariant in M_i $(i=1,2,\cdots)$ and A_i^* its adjoint in M_i.

Then for

$$\Delta = \Big\{ f = \sum_{i=1}^{\infty} f_i \in H : \sum_{i=1}^{\infty} \|A_i f_i\|^2 < \infty$$

$$\text{and} \sum_{i=1}^{\infty} \|A_i^* f_i\|^2 < \infty \Big\}$$

there exists one, and only one, closed operator A, generally unbounded, which is Δ-simple and coincides with A_i on each M_i. Its domain is the set of the elements $f \in H$ such that

$$\sum_{i=1}^{\infty} \|A_i f_i\|^2 < \infty.$$

and for these f

$$Af = \sum_{i=1}^{\infty} A_i f_i.$$

Proof: It is obvious that the operator A is linear and its domain is dense in H, because it contains all the sums of the form

$$\sum_{i=1}^{n} f_i, \quad f_i \in M_i.$$

We show, first, that the operator A is closed. In fact for $\varphi_r \to \varphi$ $(\varphi_r \in D_A)$ and $A\varphi_r \to \psi$ with

$$\varphi_r = \sum_{i=1}^{\infty} \varphi_{r_i}, \quad \varphi = \sum_{i=1}^{\infty} \varphi_i \quad \text{and} \quad \psi = \sum_{i=1}^{\infty} \psi_i$$

one has

$$\lim_{r\to\infty} \sum_{i=1}^{\infty} A_i \varphi_{r_i} = \sum_{i=1}^{\infty} \psi_i$$

then for $g_j \in M_j$

$$\Big(\lim_{r\to\infty} \sum_{i=1}^{\infty} A_i \varphi_{r_i}, \; g_j \Big)$$

$$= \lim_{r\to\infty} (A_j \varphi_{r_j}, \; g_j) = (\psi_j, \; g_j).$$

Since $\varphi_r \to \varphi$, $\varphi_{r_j} \to \varphi_j$ results and, by the boundedness of A_j in M_j, $A_j \varphi_{r_j} \to A_j \varphi_j$,

and hence

$$\lim_{r\to\infty} (A_j \varphi_{r_j} g_j) = \Big(\lim_{r\to\infty} A_j \varphi_{r_j}, \; g_j \Big)$$

$$= (A_j \varphi_j, \; g_j) = (\psi_j, g_j)$$

which implies that

$$\sum_{i=1}^{\infty} \|A_i \varphi_i\|^2 = \sum_{i=1}^{\infty} \|\psi_i\|^2 < \infty;$$

hence $\varphi \in D_A$ and $A\varphi = \psi$, so that A is a closed operator.

The fact that the operator, with dense domain, is closed implies, in a Hilbert space, that it admits an adjoint.

We define the operator T by the relations

$$Tf = \sum_{i=1}^{\infty} A_i^* f_i$$

$$D_T = \Big\{ f = \sum_{i=1}^{\infty} f_i \in H : \sum_{i=1}^{\infty} \|A_i^* f_i\|^2 < \infty \Big\};$$

we show that $T=A^*$.

It is obvious that the domain of T is dense in H and besides $\overline{D_A \cap D_T} = H$.

For $f \in D_A$ and $g \in D_T$

$$(Af,g)=\sum_{i=1}^{\infty}(A_i f_i, g_i)$$

$$=\sum_{i=1}^{\infty}(f_i, A_i^* g_i)=(f,Tg),$$

so that $T\subseteq A^*$.

Conversely, for $f\in D_A$ and $g\in D_{A^*}$, by

$$(Af,g)=(f,A^*g)$$

it follows that

$$\sum_{i=1}^{\infty}(A_i f_i, g_i)=\sum_{i=1}^{\infty}(f_i, (A^*g)_i).$$

If, particularly, we choose $f=f_j$, i.e., $f\in M_j$, we have

$$(f_j, A_j^* g_j)=(A_j f_j, g_j)=(f_j, (A^*g)_j);$$

hence $A^*g=\Sigma_{i=1}^{\infty}A_i^* g_i$, i.e., $A^*\subseteq T$, that is, $A^*=T$.

It remains to prove that the operator A is Δ-simple. If B is a closed operator such that

$$A\supseteq B\supseteq A/\Delta,$$

it is obvious that each element $\Sigma_{i=1}^{n}f_i$ belongs to D_B and

$$B\sum_{i=1}^{n}f_i=A\sum_{i=1}^{n}f_i.$$

If $f\in D_A$,

$$f=\lim_{n\to\infty}\sum_{i=1}^{n}f_i$$

and

$$Af=\lim_{n\to\infty}\sum_{i=1}^{n}A_i f_i=\lim_{n\to\infty}B\sum_{i=1}^{n}f_i;$$

since B is closed,

$$f\in D_B \quad \text{and} \quad Bf=Af$$

so that $B=A$.

In analogous way we can prove that A^* is Δ-minimal and so A is a Δ-simple operator.

In order to complete the proof, it remains only to prove the uniqueness of the operator A.

Let A' be a Δ-simple operator which coincides with A_i on M_i. Since A' is closed it is necessarily defined for all the elements f such that the series $\Sigma_{i=1}^{\infty}A' f_i$ is convergent and the sum of this series is equal to Af.

Since $Af_i=A_i f_i$ and the convergence of a series of orthogonal elements is equivalent to the convergence of the series of the squares of their norms, the set of these vectors f coincides with D_A and

$$Af=Af,$$

i.e.,

$$A'\supseteq A.$$

The statement follows from the Δ-maximality of A.

[1] $B(H)$ is the well known *-algebra of bounded operators in Hilbert space H. For the matrix representation of its operators see, for instance, (a) N.I. Akhiezer and I.M. Glazman, *Theory of Linear Operators in Hilbert Space* (Ungar, New York, 1961), Vol. I. (b) V.I. Smirnov, *A Course of Higher Mathematics* (Pergamon, New York, Oxford, London, 1964), Vol. V.

[2] C_D is a *-algebra of unbounded operators. For the definitions and properties of C_D, see: R. Ascoli, G. Epifanio, and A. Restivo, Commun. Math. Phsy. **18**, 291 (1970); Riv. Mat. Univ. Parma **3**, 21 (1974); G. Lassner, Rep. Math. Phys. **3**, 279 (1972) [the *-algebra C_D is called $L_c(D)$ by Lassner]. The theory of matrix representation of operators of C_D has been given by one of the authors of this paper in G. Epifanio, J. Math. Phys. **17**, 1688 (1976).

[3] We call weak topology of the space H (or D) the topology defined by the set of seminorms
$\{\varphi\to|(\varphi,\psi)|/\psi\in H \text{ (or } D)\}$.

[4] See, for instance, M.H. Stone, *Linear Transformations in Hilbert Space* (American Mathematical Society, New York, 1966), Chap. III, §1, Theorem 3.1.

[5] See, for instance, Ref. 4, Chap. III, §1, Theorem 3.3.

[6] See J. von Neumann, Math. Ann. **102/1**, 49 (1929); J. Math. **161**, 208 (1929). Various books report the von Neumann's theory of matrix representation of closed symmetric operators. See, for instance, Ref. 1(a), Sec. 47 and Ref. 1(b), §3.

[7] The operator R is defined on the basis vector by the relations $Re_\nu=\Sigma_{\mu}' {}_1 A_{\mu\nu}e_\mu$ and extended by linearity to the linear envelope $\{e_\nu\}^l$.

[8] One uses for this topology the notation $\sigma(E,F)$.

[9] For the proof see N. Bourbaki, *Elements de Mathématique: Espaces Vectoriels Topologiques* (Hermann, Paris, 1965), 2nd ed., Chap. II, §6, Prop. 5 and corollary.

[10] It is known that the proof of this theorem is usually made by means of the generalized closure equation. Hence this is a confirmation that the existence of the adjoint operator is equivalent to the continuity stated in the Theorem 1.

[11] Both the operators T and T' are closed. See Ref. 4, Chap. III, Theorem 3.2.

[12] This theorem reduces to that of Riesz and Lorch if A is self-adjoint. See F. Riesz and B. Sz.Nagy, *Leçons d'analyse fonctionelle* (Gauthier-Villars, Paris, 1972), Chap. VIII, n. 120.

Wigner coefficients for SU(6)⊃SU(3)⊗SU(2)[a]

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A technique for evaluating the Wigner coeficients for SU(6) with the physically interesting subgroups SU(3)⊗SU(2) is outlined. Coefficients appropriate for coupling a single quark to a many quark wavefunction are tabulated for functions of nine or fewer quarks.

I. INTRODUCTION

The SU(6) nonrelativistic quark model[1] has proven to be remarkably successful in organizing the hadronic particles into multiplets and accounting for many of the observed decay rates. The SU(6) group also appears in some relativistic quark models, such as the bag model,[2,3] in those cases in which the quarks are assumed to be S wave and their total angular momentum is only the intrinsic spin. The calculation of masses and the decay channels of multiquark and quark antiquark states may require Wigner and recoupling coefficients which are the generalization to SU(6) of the well-known Wigner (Clebsch–Gordan) and Racah coefficient of the rotation group. These coefficients have not previously been calculated, save for a very few special cases.[3,4]

Ideally, closed, analytic expressions would be available for the SU(6)⊃SU(3)⊗SU(2) Wigner coefficients, as in the familiar case of the rotation group, or for the SU(3)⊃SU(2) group.[5,6] However, severe mathematical difficulties make this prospect at the moment merely a pious hope. The unique specification of a state belonging to an irreducible representation of a unitary group SU(n) requires $\frac{1}{2}n(n-1)$ labels in addition to the $n-1$ quantities which specify the irreducible representation. These latter quantities may be chosen as the eigenvalues of the $n-1$ invariants, of which the first is the familiar Casimir operator.

In the so-called canonical chain of groups, viz.,

$$\mathrm{SU}(n)\supset\mathrm{SU}(n-1)\supset\cdots\supset\mathrm{SU}(1), \tag{1}$$

the additional labels are given by the labels of each of the subgroups, and as a whole comprise the Gel'fand–Tsetlin pattern.[7] When the subgroups are not those of the canonical chain, the subgroups do not provide an adequate number of labels with which to specify a state uniquely. Two examples of noncanonical chains familiar to physicists are SU(4) ⊃SU(2)⊗SU(2) (the Wigner supermultiplet model[8]) and SU(6)⊃SU(3)⊗SU(2). A third possibility is SU(8)⊃SU(4)⊗SU(2), which might arise were a charmed quark added to the three more usual quarks.

The mathematical difficulty is clear if one considers labelling a state which is an irreducible representation of SU($2m$)⊃SU(m)⊗SU(2). A state belonging to an irreducible representation of SU($2m$) requires $m(2m-1)$ labels. The SU(2) subgroup provides two labels, namely the total angular momentum or spin S, and its projection on the z axis. The SU(m) subgroup provides an additional $m-1$ labels which specify the irreducible representation of SU(m) plus the $\frac{1}{2}m(m-1)$ labels from the subgroups of SU(m), or a total of $\frac{1}{2}(m+2)(m-1)$ labels. Hence, the subgroups of SU($2m$) provide in total only $\frac{1}{2}(m+2)(m-1)+2$ labels, and one must find 2, 8, and 17 *additional* operators in the case of the SU(4), SU(6), and SU(8) groups, respectively.

The two additional operators in the SU(4)⊃SU(2) ⊗SU(2) example have been found by Moshinsky and Nagel,[9] but they do not lend themselves easily to calculations, being quadratic and cubic functions of the generators of the group. It is unlikely one might find eight simple operators for SU(6)⊃SU(3)⊗SU(2).

An additional complication occurs because the Kronecker product of two representations of SU(6) is in general not simply reducible. In the product

$$[f_1]\times[f_2]=\sum_{[f]} n_f[f], \tag{2}$$

which for the SU(2) group is just the Clebsch–Gordan series, n_f is the outer multiplicity and may be greater than one, although this never occurs if either $[f_1]$ or $[f_2]$ represents a single quark or antiquark state. The resulting states belonging to the irreducible representation $[f]$ are not automatically orthogonal. It is conceivable that an orthogonal combination may be chosen using a generalization of a technique suggested by Moshinsky[10] for the SU(3) group; such an approach is assuredly involved and not amendable to analytic calculations.

Because of these difficulties, it appears inappropriate to attempt a purely analytic solution for the Wigner and Racah coefficients of SU(6)⊃SU(3)⊗SU(2). [The simpler case of SU(4)⊃SU(2)⊗SU(2) has been investigated by Hecht and Pang[11]); the reader is advised to refer thereto to grasp the magnitude of the difficulties, even in the case of the simpler SU(4) representations.] Instead, a recursive approach is proposed which is amenable to numerical calculations, but has the disadvantage that it is purely numerical and as such involves often arbitrary choices of phases (although the Young–Yamanouchi choice of phases is maintained) and arbitrary orthogonalization of basis states in those cases where there is outer multiplicity.

In Sec. 2 the SU(6)⊃SU(3)⊗SU(2) Wigner coefficient is defined and necessary notation introduced. In Sec. 3 the method of calculation is presented, and in Sec. 4 questions of phase and the construction of antisymmetric wavefunctions are explored. Examples are given in Sec. 5.

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2. THE SU(6) ⊃ SU(3) ⊗ SU(2) WIGNER COEFFICIENT

The technique used in this paper exploits the intimate relationship between the unitary groups and the symmetric group[12] and is a generalization of the technique used by Jahn[13] to evaluate coefficients of fractional parentage employed in calculations using the nuclear shell model. An N-quark wavefunction characterized by an irreducible representation of SU(6) describes the symmetry of the wavefunction under the permutation of the quarks. It is, therefore, simultaneously a representation of the symmetric group S_N.

An irreducible representation of SU(n) will be denoted by the n labels $[h_i]=[h_1\cdots h_n]$ which characterize a Young partition of N with at most n rows. Since a column of n boxes transforms as a scalar under SU(n), it is more convenient to label the irreducible representations using the $n-1$ labels

$$f_i=h_i-h_{i+1},\ i<n. \tag{3}$$

For SU(2), this leaves one label,

$$f_1=h_1-h_2=2S; \tag{4}$$

for SU(3), the two labels

$$\lambda=h_1-h_2,\quad \mu=h_2-h_3 \tag{5}$$

will be denoted by $(\lambda\mu)$. The dimension of a representation of SU(3) is

$$g(\lambda\mu)=\tfrac{1}{2}(\lambda+1)(\mu+1)(\lambda+\mu+2) \tag{6}$$

and the more familiar (to particle physicists), but nonunique, notation is regained. The representations of SU(6) and S_n will be given by $[f_1f_2\cdots f_5]$ and $[h_1\cdots h_6]$, respectively, where

$$N=\sum_{i=1} h_i=\sum_{i=1} if_i+6k,\ k=\text{integer}. \tag{7}$$

Expressions for the Casimir operator of SU(n) are given in the Appendix.

A state belonging to an irredudible representation $[f_1\cdots f_5]$ of SU(6) will be denoted by

$$\begin{matrix}\text{SU(6)}\to\\ \text{SU(3)}\times\text{SU(2)}\to\end{matrix}\left|\begin{matrix}[f_1\cdots f_5\ ]\\ (\lambda\ \mu)\quad S\omega\\ I\ I_z\ Y\ m_s\end{matrix}\right\rangle \tag{8}$$

where m_S is the z projection of the spin S and I, I_z, and Y are subgroup labels of SU(3). If the SU(3) group in Eq. (8) describes the flavor degrees of freedom, then I, I_z, and Y are the isospin, its z projection and hypercharge, respectively. The Wigner coefficients of SU(6) ⊃ SU(3) ⊗ SU(2) are independent of the subgroup labels of SU(3) and SU(2) and any convenient choice may be made. Obviously, the SU(6) coefficients are also independent of whether the SU(3) group in the state (8) describes color, flavor or some other degree of freedom. The label ω denotes the eight additional quantum numbers necessary to uniquely specify the state; as these are not known, we shall allow ω to run from 1 to r, where r is the degeneracy which would otherwise result. The quantity ω is first needed in the five quark system with SU(6) representation [311].

The SU(6) ⊃ SU(3) ⊗ SU(2) Wigner coefficient reduces the product of two states such as (8) above to a third state which also belongs to an irreducible representation of SU(6) ⊃ SU(3) ⊗ SU(2):

$$\left|\begin{matrix}[f_1\cdots f_5\ ]\\ (\lambda\ \mu)S\ \omega\\ I\ I_z\ Y\ m_s\end{matrix}\right\rangle=\left[\left|\begin{matrix}[f^{(1)}]\\ \cdots\end{matrix}\right\rangle\left|\begin{matrix}[f^{(2)}]\\ \cdots\end{matrix}\right\rangle\right]^{[f](\lambda\mu)S\omega}_{I\ I_z\ Y\ m_s\ \rho}$$

$$=\sum_{\substack{(\lambda_1\mu_1)S_1\omega_1\\(\lambda_2\mu_2)S_2\omega_2}}\left\langle\begin{matrix}[f_1] & [f_2] & [f_2]\\ (\lambda_1\mu_1)\ S_1\omega_1 & (\lambda_2\mu_2)\ S_2\omega_2 & (\lambda\ \mu)S\ \omega\end{matrix}\right\rangle$$

$$\times\left[\left|\begin{matrix}[f^{(1)}]\\ (\lambda_1\mu_1)S_1\omega_1\end{matrix}\right\rangle\left|\begin{matrix}[f^{(2)}]\\ (\lambda_2\mu_2)S_2\omega_2\end{matrix}\right\rangle\right]^{(\lambda\mu)S\omega}_{I\ I_z Y m_s} \tag{9}$$

$$=\sum_{\substack{(\lambda_1\mu_1)S_1\omega_1)\\(\lambda_2\mu_2)S_2\omega_2)}}\left\langle\begin{matrix}[f^{(1)}] & [f^{(2)}] & [f]\\ (\lambda_1\mu_1)S_1\omega_1 & (\lambda_2\mu_2)S_2\omega_2 & (\lambda\ \mu)S\omega\end{matrix}\right\rangle$$

$$\times\sum_{\substack{\rho\ I_1 I_{1z} Y_1\\ I_2 I_{2z} Y_2}}\left\langle\begin{matrix}(\lambda_1\mu_1) & (\lambda_2\mu_2) & (\lambda\ \mu)\\ I_1\ I_{1z}\ Y_1 & I_2\ I_{2z}\ Y_2 & I\ I_z\ Y\end{matrix}\right\rangle_\rho \tag{10}$$

$$\sum_{m_1m_2}\langle S_1S_2m_1m_2\,|\,Sm_s\rangle\left|\begin{matrix}[f^{(1)}]\\ (\lambda_1\mu_1)S_1\omega_1\\ I_1I_{1z}Y_1\end{matrix}\right\rangle\left|\begin{matrix}[f^{(2)}]\\ (\lambda_2\mu_2)S_2\omega_2\\ I_2I_{2z}Y_2\end{matrix}\right\rangle.$$

The label ρ distinguishes orthogonal states in those cases in which there is outer multiplicity as may occur in the Kronecker products of two SU(6) or two SU(3) representations, Eq. (2).

The second and third factors in Eq. (10) are the SU(3) Wigner coefficients[6,14] and the SU(2) Wigner (Clebsch–Gordan) coefficients, respectively. The first factor is the so-called SU(6) ⊃ SU(3) ⊗ SU(2) isoscalar factor and may be identified as the SU(6) ⊃ SU(3) ⊗ SU(2) Wigner coefficient. In Eq. (9) the product state is coupled to an irreducible representation of SU(3) and SU(2), but *not* SU(6). It will form the basis of much that follows. In this paper we shall calculate the SU(6) Wigner coefficient for the coupling of a single quark with representation (10)1/2 to an $N-1$ quark state. The calculation may then be extended to the coupling of several quarks to several quarks or anti-quarks in the usual manner.[15]

3. THE EVALUATION OF THE COEFFICIENTS

As mentioned in Sec. 2, the calculation exploits the intimate connection between the representations of SU(6) and the symmetric group on N objects S_N. The properties of the symmetric group are well documented.[12,16]. Of essential interest herein is that the operator

$$P^N=\sum_{i=j} P_{ij}, \tag{11}$$

where P_{ij} permutes particles i and j, is diagonal between representations of S_N, and has the eigenvalue

$$\langle [h_1 \cdots h_6\ ] | P^N | [h'_1 \cdots h'_6] \rangle$$
$$= \tfrac{1}{2}\left[\sum_i h_i^2 - \sum_i \tilde{h}_i^2\right] \delta([h_i],[h'_i]) \equiv C([h_i]). \quad (12)$$

In Eq. (12) $[\tilde{h}_i]$ is the conjugate representation of $[h_i]$ and is found simply by interchanging the rows and columns of the Young diagram for $[h_i]$. From the preceeding discussion it is evident that P^N is also diagonal in SU(6). Hence, to obtain the Wigner coefficients of $SU(6) \supset SU(3) \otimes SU(2)$, it suffices to diagonalize P^N in a basis labeled by representation of SU(3) and SU(2); the components of the resultant eigenvectors will be just the desired Wigner coefficients.

It remains to calculate the matrix of P^N in the basis specified by the state of Eq. (9) in the case for which $[f^{(1)}]$ represents an $N-1$ quark state and $[f^{(2)}] = [1]$, a state of a single quark.

$$\left\langle q^{N-1} \begin{matrix}[h^{(1)}] \\ (\lambda_1\mu_1)S_1\omega_1\end{matrix} \times q \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} ;\ (\lambda\mu)S\omega \left| \sum_{i<j} P_{ij} \right| q^{N-1} \begin{matrix}[h^{(1)}] \\ (\bar{\lambda}_1\bar{\mu}_1)\bar{S}_1\bar{\omega}_1\end{matrix} \times q \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} ;(\lambda\mu)S\omega \right\rangle = \delta_{\lambda_1\bar{\lambda}_1}\delta_{\mu_1\bar{\mu}_1}\delta_{\omega_1\bar{\omega}_1} C([h_i^{(1)}])$$
$$+(N-1)\left\langle \begin{matrix}[h^{(1)}] \\ (\lambda_1\mu_1)S_1\omega_1\end{matrix} \times \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} ;\ (\lambda\mu)S\omega \left| P_{n-1,n} \right| \begin{matrix}[h^{(1)}] \\ (\bar{\lambda}_1\bar{\mu}_1)\bar{S}_1\bar{\omega}_1\end{matrix} \times \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} ;\ (\lambda\mu)S\omega \right\rangle. \quad (13)$$

Note that the states in Eq. (13) are labelled by the representations of S_N, which are, however, simply related to the SU(6) representations in a one to one manner through Eq. (7).

The matrix elements of the transposition operator $P_{n-1,n}$ in the second term of Eq. (13) may be evaluated by using $SU(6) \supset SU(3) \otimes SU(2)$ Wigner coefficients to decompose a state of $N-1$ quarks into the product of state of $N-2$ quarks and a single-quark state, and recoupling the SU(2) and SU(3) representations separately:

$$\left\langle \begin{matrix}[f^{(1)}] \\ (\lambda_1\mu_1)S_1\omega_1\end{matrix} \times \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} (\lambda\mu)S\omega \left| P_{n-1,n} \right| \begin{matrix}[f^{(1)}] \\ (\bar{\lambda}_1\bar{\mu}_1)\bar{S}_1\bar{\omega}_1\end{matrix} \times \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} ;\ (\lambda\mu)S\omega \right\rangle$$
$$= \sum_{(\lambda''\mu'')S''\omega''} \left\langle \begin{matrix}[f''] \\ (\lambda''\mu'')S''\omega''\end{matrix} \times \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} \left| \begin{matrix}[f^{(1)}] \\ (\lambda_1\mu_1)S_1\omega_1\end{matrix} \right\rangle \left\langle \begin{matrix}[f''] \\ (\lambda''\mu'')S''\omega''\end{matrix} \begin{matrix}[1] \\ (10)\,\frac{1}{2}\end{matrix} \left| \begin{matrix}[f^{(1)}] \\ (\bar{\lambda}_1\bar{\mu}_1)S_1\bar{\omega}_1\end{matrix} \right\rangle \right.$$
$$\times (-1)^{1+S_1+\bar{S}_1} \begin{Bmatrix} S_1 & S'' & \frac{1}{2} \\ \bar{S}_1 & S & \frac{1}{2} \end{Bmatrix} (-1)^{\lambda_1+\mu_1+\bar{\lambda}_1+\bar{\mu}_1+\lambda+\mu+\lambda''+\mu''} U[(10)(\lambda''\mu'')(10)(\lambda\mu);\bar{\lambda}_1,\bar{\mu}_1)(\lambda_1\mu_1)\ ]. \quad (14)$$

In Eq. (14) $U(\cdots)$ is a unitary Racah coefficient[6] for the SU(3) group. Analytic expressions for the SU(3) Racah coefficints needed for evaluating Eq. (14) may be readily obtained by using

$$U[(10)(\lambda''\mu'')(\lambda\mu)(10);(\lambda_2\mu_2)(\lambda_1\mu_1)] = (-1)^{\lambda''+\mu''+\lambda+\mu+\lambda_1+\mu_1+\lambda_2+\mu_2}$$
$$\times \sum_{(\lambda_{23}\mu_{23})} U[(\lambda''\mu'')(10)(\lambda\mu)(10);(\lambda_2\mu_2)(\lambda_{23}\mu_{23})\ ]$$
$$\times U[(\lambda''\mu'')(10)(\lambda\mu);(\lambda_1\mu_1)(\lambda_{23}\mu_{23})\ ](-1)^{\mu_{23}}. \quad (15)$$

Expressions for the Racah coefficients appearing on the right-hand side of Eq. (15) have been given by Vergados.[17] The resultant Racah coefficients are given in Table I.

The matrix of $P_{n,n-1}$ may be constructed using Eq. (14) for a specified $(\lambda\mu)S$ and $[f^{(1)}]$ using all possible $(\lambda_1\mu_1)S_1$ belonging to $[f^{(1)}]$ which will connect with $(\lambda\mu)S$. The matrix is then diagonalized; the resulting eigenvectors which are—up to a phase—just the required $SU(6) \supset SU(3) \otimes SU(2)$ Wigner coefficients may be identified with the appropriate irreducible representation of S_n, and hence SU(6), by virtue of Eq. (12). It is apparent that this procedure defines a recursive procedure; to calculate the Wigner coefficients for a state of N quarks, it is necessary to calculate the coefficients for $N-1$ quarks, and so on. However, it does have the virtue that it resolves the problem of the multiplicity. If a Jacobi diagonalization procedure is used, eigenvectors corresponding to degenerate eigenvalues are automatically orthogonal. This is a nontrivial advantage; the multiplicity is already six for the nine-quark state [531](22)3/2 and increases rapidly with an increasing number of quarks.

An alternative, but equivalent procedure would have been to diagonalize the Casimir operator of SU(6), an approach which would closely parallel the technique of Bayman and Lande[18] to evaluate fractional parentage coefficients for l^N and j^N configurations of fermions.

4. CONSTRUCTION OF TOTALLY ANTISYMMETRIC WAVEFUNCTIONS;CHOICE OF PHASES

The expansion of a totally antisymmetric wavefunction of n fermions as a sum over the product a state of $n-1$ fermions and a one-fermion state was introduced by Racah,[19] and the coefficients in the expansion were known as coefficients of fractional parentage. In the case that the n-fermion state is labelled by irreducible representations of some group, then the coefficients of fractional parentage may be identified with the Wigner coefficients of that group.

It will be assumed for convenience that the quark wave-

TABLE I. The SU(3) Racah coefficients necessary for the evaluation of Eq. (14).

$U[(10)(\lambda\mu)(\lambda'\mu')(10);(\lambda_{12}\mu_{12})(\lambda_{13}\mu_{13})]$

$(\lambda'\mu')=(\lambda\mu+1)$

$(\lambda_{12}\mu_{12})$ \ $(\lambda_{13}\mu_{13})$	$(\lambda+1\ \mu)$	$(\lambda-1\ \mu+1)$
$(\lambda+1\ \mu)$	$\frac{1}{\lambda+1}$	$\frac{\sqrt{\lambda(\lambda+2)}}{\lambda+1}$
$(\lambda-1\ \mu+1)$	$\frac{\sqrt{\lambda(\lambda+2)}}{\lambda+1}$	$-\frac{1}{\lambda+1}$

$(\lambda'\mu')=(\lambda+1\ \mu-1)$

$(\lambda_{12}\mu_{12})$ \ $(\lambda_{13}\mu_{13})$	$(\lambda+1\ \mu)$	$(\lambda\ \mu-1)$
$(\lambda+1\ \mu)$	$-\frac{1}{\lambda+\mu+2}$	$\frac{\sqrt{(\lambda+\mu+1)(\lambda+\mu+3)}}{\lambda+\mu+2}$
$(\lambda\ \mu-1)$	$\frac{\sqrt{(\lambda+\mu+1)(\lambda+\mu+3)}}{\lambda+\mu+2}$	$\frac{1}{\lambda+\mu+2}$

$(\lambda'\mu')=(\lambda-1\ \mu)$

$(\lambda_{12}\mu_{12})$ \ $(\lambda_{13}\mu_{13})$	$(\lambda\ \mu-1)$	$(\lambda-1\ \mu+1)$
$(\lambda\ \mu-1)$	$-\frac{1}{\mu+1}$	$\frac{\sqrt{\mu(\mu+2)}}{\mu+1}$
$(\lambda+1\ \mu+1)$	$\frac{\sqrt{\mu(\mu+2)}}{\mu+1}$	$\frac{1}{\mu+1}$

Other allowed coefficients: $U[\cdots]=+1$.

function is specified by the irreducible representations of $SU(3)_f$ and $SU(6)\supset SU(3)_c\otimes SU(2)$, where the subscripts f and c denote flavor and color, respectively. If quarks carrying other quantum numbers such as charm or beauty are included, then $SU(3)_f$ must be generalized to a larger unitary group. This would not affect any of the discussion below save for Eq. (18a). The totally antisymmetric state of n quarks is

$$\Psi(q^n[h_1\cdots h_6\ ](\lambda_c\mu_c)S\omega\Lambda\nu,(\lambda_f\mu_f)I\ I_z\ Y)$$

$$=(n_A)^{-1/2}\sum_{(r)}\Phi(q^n[h_1\cdots h_6\ ](\lambda_c\mu_c)\times S\omega\epsilon\Lambda\nu,(r)\ )\chi(q^n(\lambda_f\mu_f)I\ I_z\ Y,(r)\ ). \tag{16}$$

The summation is over the n_k Yamanouchi symbols (r) allowed by the irreducible representation $[h_1\cdots h_6]$ of S_n; n_h is the dimension of $[h_1\cdots h_6]$.

A sufficient condition that the total wave function be antisymmetric is for ϕ and χ to transform contragradiently with respect to one another under permutations of the n quarks. [Note that this differs from certain authors, e.g., Hammermesh,[16] who assume ϕ and χ transform in the same way; in this case one must insert an additional phase of $(-)^{P_{(r)}}$ into Eq. (16).] The requirement that $(\lambda_f\mu_f)$ be conjugate to $[h_1\cdots h_6]$:

$$[g_1g_2g_3]\equiv(\lambda_f\mu_f)=[h_1\cdots h_6] \tag{17}$$

immediately gives the restrictions

$$h_i\leqslant 3,\quad i=1-6, \tag{18a}$$

$$g_i\leqslant 6,\quad i=1,2,3. \tag{18b}$$

The first of these restrictions, Eq. (18a), is only ture in the event that $SU(3)_f$ is the group conjugate to SU(6). If $SU(3)_f$ is enlarged to encompass further quantum numbers, then the restriction is correspondingly less severe. For this reason no restriction on the h_i was imposed (for less than nine quarks) when the SU(6) Wigner coefficients were calculated.

The decomposition of ψ into a product of an $(n-1)$-quark wavefunction and a one-quark wavefunction may now be performed by applying the relevant Wigner coefficients on ϕ and χ separately. The SU(3) Wigner coefficients may be taken from the tabulations of de Swart[14] or calculated with available computer routines.[20] The SU(6) coefficients are those of Table II.

TABLE II. The SU(6)⊃SU(3)⊗SU(2) Wigner coefficients. The SU(6) representations are arranged in order of descending value of $C([h])$, Eq. (12) and the SU(3)⊗SU(2) representations in descending order of the SU(3) Casimir operator and ascending value of S.

$q^3\to q^2$		[2]		[11]	
		(20)1	(01)0	(20)0	(01)1
[3]	$(30)\frac{3}{2}$	1	0		
	$(11)\frac{1}{2}$	$1/\sqrt{2}$	$1/\sqrt{3}$		
[21]	$(30)\frac{1}{2}$	1	0	−1	0
	$(11)\frac{1}{2}$	$1/\sqrt{2}$	$-1/\sqrt{2}$	$1/\sqrt{2}$	$1/\sqrt{2}$
	$(11)\frac{3}{2}$	1	0	0	−1
	$(00)\frac{1}{2}$	0	1	0	1
[111]	$(11)\frac{1}{2}$			$1/\sqrt{2}$	$-1/\sqrt{2}$
	$(00)\frac{3}{2}$			0	1

$q^4\to q^3$		[21]				[111]	
		$(30)\frac{1}{2}$	$(11)\frac{1}{2}$	$(11)\frac{3}{2}$	$(00)\frac{1}{2}$	$(11)\frac{1}{2}$	$(00)\frac{3}{2}$
[22]	(40)0	1					
	(21)1	$1/\sqrt{2}$	$1/\sqrt{3}$	$1/\sqrt{3}$			
	(02)0		1				
	(02)2			1			
	(10)1		$1/\sqrt{3}$	$-1/\sqrt{3}$	$-1/\sqrt{3}$		
[211]	(21)0	$1/\sqrt{2}$	$-1/\sqrt{2}$			−1	
	(21)1	$1/\sqrt{2}$		$-1/\sqrt{2}$		1	
	(02)1		$1/\sqrt{2}$	$-1/\sqrt{2}$		−1	
	(10)0		$+1/\sqrt{2}$		$-1/\sqrt{2}$	−1	
	(10)1		$+\sqrt{2/3}$	$+1/\sqrt{6}$	$+1/\sqrt{6}$	$1/\sqrt{3}$	$-\sqrt{2/3}$
	(10)2			1			1
[1111]	(02)0					1	
	(10)1					$\sqrt{2/3}$	$\sqrt{1/3}$

TABLE II. (*Continued*)

$q^4 \to q^3$	[3]		[21]			
[4]						
(40)2	1		—	—	—	—
(21)1	$\sqrt{1/3}$	$\sqrt{2/3}$	—	—	—	—
(02)0		1	—	—	—	—
[31]						
(40)1	1		-1			
(21)0		1	$-1/\sqrt{2}$	$-\sqrt{1/2}$		
(21)1	$\sqrt{2/3}$	$-\sqrt{1/3}$	$1/\sqrt{6}$	$-\sqrt{2/3}$	$1/\sqrt{6}$	
(21)2	1				-1	
(02)1		1		$-1/\sqrt{2}$	$-1/\sqrt{2}$	
(10)0		1		$1/\sqrt{2}$		$1/\sqrt{2}$
(10)1		1			$1/\sqrt{2}$	$-1/\sqrt{2}$

$q^5 \to q^4$	[4]			[31]						
	(40)2	(21)1	(02)0	(40)1	(21)0	(21)1	(21)2	(02)1	(10)0	(10)1
[5]										
$(50)\frac{5}{2}$	1									
$(31)\frac{3}{2}$	$\frac{1}{2}$	$\sqrt{3/2}$								
$(12)\frac{1}{2}$		$\sqrt{3/5}$	$\sqrt{2/5}$							
[41]										
$(50)\frac{3}{2}$	1			-1						
$(31)\frac{1}{2}$		1		$-\sqrt{1/3}$	$-\sqrt{8/15}$	$-\sqrt{2/15}$				
$(31)\frac{3}{2}$	$\sqrt{3/2}$	$-\frac{1}{2}$		$1/\sqrt{12}$	0	$-\sqrt{5/6}$	$1/\sqrt{12}$			
$(31)\frac{5}{2}$	1						-1			
$(12)\frac{1}{2}$		$\sqrt{2/5}$	$-\sqrt{3/5}$	0	$1/\sqrt{3}$	$-1/\sqrt{3}$	0	$1/\sqrt{3}$		
$(12)\frac{3}{2}$		1				$-\sqrt{2/15}$	$-1/\sqrt{3}$	$-\sqrt{8/15}$		
$(20)\frac{1}{2}$		1			$1/\sqrt{30}$	$\sqrt{3/10}$			$-1/\sqrt{2}$	$1/\sqrt{6}$
$(20)\frac{3}{2}$		1					$1/\sqrt{3}$			$-\sqrt{2/3}$
$(01)\frac{1}{2}$			1					$1/\sqrt{5}$	$-1/\sqrt{5}$	$-\sqrt{3/5}$

TABLE II. (*Continued*)

$q^5 \to q^4$	[31] (40)1	(21)0	(21)1	(21)2	(02)1	(10)0	(10)1	[22] (40)0	(21)1	(02)2	(01)2	(10)1
[32] $(50)\frac{1}{2}$	1							1				
$(31)\frac{1}{2}$	$1/\sqrt{6}$	$-\sqrt{5/12}$	$\sqrt{5/12}$					$-\sqrt{3/8}$	$-\sqrt{5/8}$			
$(31)\frac{3}{2}$	$\sqrt{5/12}$		$1/\sqrt{6}$	$\sqrt{5/12}$					1			
$(12)\frac{1}{2}$		$1/\sqrt{6}$	$\sqrt{2/3}$		$1/\sqrt{6}$				1/2	$\sqrt{3/2}$		
$(12)\frac{3}{2}$			$\sqrt{5/12}$	$1/\sqrt{6}$	$-\sqrt{5/12}$				$-\sqrt{5/8}$		$-\sqrt{3/8}$	
$(12)\frac{5}{2}$				1							1	
$(20)\frac{1}{2}$		$\sqrt{5/12}$				1/2	$1/\sqrt{3}$		$-\sqrt{5/8}$			$\sqrt{3/8}$
$(20)\frac{3}{2}$			$\sqrt{3/8}$	$-\sqrt{5/12}$			$-\sqrt{5/24}$		1/4			$\sqrt{15/4}$
$(01)\frac{1}{2}$					$1/\sqrt{2}$	$1/\sqrt{2}$				$-1/2$		$-\sqrt{3/2}$
$(01)\frac{3}{2}$					1/2		$\sqrt{3/2}$				$-\sqrt{5/8}$	$\sqrt{3/8}$

TABLE II. (*Continued*)

	[31]							[211]					
$q^5 \to q^4$	(40)1	(21)0	(21)1	(21)2	(02)1	(10)0	(10)1	(21)0	(21)1	(02)1	(10)0	(10)1	(10)2
$[311](31)\frac{1}{2}$	$1/\sqrt{2}$	$-1/\sqrt{20}$	$-\sqrt{9/20}$					$\sqrt{3/2}$	$-\frac{1}{2}$				
$(31)\frac{3}{2}$	$1/\sqrt{2}$			$-1/\sqrt{2}$					1				
$(12)\frac{1}{2}$		$1/\sqrt{2}$			$-1/\sqrt{2}$			$\sqrt{3/10}$	$\sqrt{2/5}$	$\sqrt{3/10}$			
$(12)\frac{3}{2}$			$\sqrt{9/20}$	$-1/\sqrt{2}$	$1/\sqrt{20}$				$-1/2$	$\sqrt{3/2}$			
$(20)\frac{1}{2}$		$\frac{1}{2}\sqrt{3/5}$	$-\sqrt{3/5}$			$-1/2$	0	$-1/2$			$-\sqrt{3/20}$	$\sqrt{3/5}$	
$(20)\frac{1}{2}$		$\sqrt{2/5}$	$1/\sqrt{10}$			0	$-1/\sqrt{2}$		$-1/\sqrt{2}$		$\sqrt{2/5}$	$\sqrt{1/10}$	
$(20)\frac{3}{2}$			$\sqrt{5/8}$	1/2			$1/\sqrt{8}$		$\sqrt{1/8}$			$\sqrt{5/8}$	$-1/2$
$(20)\frac{5}{2}$				1									1
$(01)\frac{1}{2}$					$\sqrt{3/10}$	$-\sqrt{3/10}$	$\sqrt{2/5}$			$1/\sqrt{2}$	$1/\sqrt{2}$		
$(01)\frac{3}{2}$					$\sqrt{3/4}$		$-1/2$			$-\sqrt{1/20}$		$\sqrt{9/20}$	$1/\sqrt{2}$

	[22]					[211]					
$q^5 \to q^4$	(40)0	(21)1	(02)0	(02)2	(10)1	(21)0	(21)1	(02)1	(10)0	(10)1	(10)2
$[221](31)\frac{1}{2}$	$\sqrt{5/8}$	$-\sqrt{3/8}$				$-1/2$	$-\sqrt{3/2}$				
$(12)\frac{1}{2}$		$\sqrt{3/2}$	$-1/2$			$-1/\sqrt{2}$		$1/\sqrt{2}$			
$(12)\frac{3}{2}$		$\sqrt{3/8}$		$-\sqrt{5/8}$			$-\sqrt{3/2}$	$-1/2$			
$(20)\frac{1}{2}$		$\sqrt{3/8}$			$\sqrt{5/8}$	1/2	$-1/\sqrt{3}$		$-\sqrt{5/12}$		
$(20)\frac{3}{2}$		$\sqrt{15/4}$			$-1/4$		$\sqrt{5/24}$			$-\sqrt{3/8}$	$-\sqrt{5/12}$
$(01)\frac{1}{2}$			$\sqrt{3/2}$		$-1/2$			$1/\sqrt{6}$	$-1/\sqrt{6}$	$-\sqrt{2/3}$	
$(01)\frac{3}{2}$				$\sqrt{3/8}$	$\sqrt{5/8}$			$-\sqrt{5/12}$		$-\sqrt{5/12}$	$1/\sqrt{6}$
$(01)\frac{5}{2}$				1							-1

TABLE II. (*Continued*)

$q^5 \to q^4$	[211] (21)0	(21)1	(02)1	(10)0	(10)1	(10)2	[1111] (02)0	(10)1
[2111] $(12)\frac{1}{2}$	$1/\sqrt{5}$	$-\sqrt{3/5}$	$+1/\sqrt{5}$				1	
$(20)\frac{1}{2}$	$1/\sqrt{2}$	$+1/\sqrt{6}$		$1/\sqrt{30}$	$\sqrt{3/10}$			1
$(20)\frac{3}{2}$		$\sqrt{2/3}$				$1/\sqrt{3}$		-1
$(01)\frac{1}{2}$			$1/\sqrt{3}$	$-1/\sqrt{3}$	$1/\sqrt{3}$		$-\sqrt{3/5}$	$-\sqrt{2/5}$
$(01)\frac{3}{2}$			$\sqrt{8/15}$		$-\sqrt{2/15}$	$1/\sqrt{3}$		1
[11111] $(01)\frac{1}{2}$							$\sqrt{2/5}$	$-\sqrt{3/5}$

TABLE II. (*Continued*)

$q^6 \to q^5$	[5] $(50)_{\frac{5}{2}}$	$(31)_{\frac{3}{2}}$	$(12)_{\frac{1}{2}}$	[41] $(50)_{\frac{3}{2}}$	$(31)_{\frac{1}{2}}$	$(31)_{\frac{3}{2}}$	$(31)_{\frac{5}{2}}$	$(12)_{\frac{1}{2}}$	$(12)_{\frac{3}{2}}$	$(20)_{\frac{1}{2}}$	$(20)_{\frac{3}{2}}$	$(01)_{\frac{1}{2}}$
[6] (60)3	1											
(41)2	$\sqrt{1/5}$	$\sqrt{4/5}$										
(22)1		2/3	$\sqrt{5/3}$									
(03)0			1									
[51] (60)2	1			-1								
(41)1		1		$-1/2$	$-5/6$	$-\sqrt{1/18}$						
(41)2	$\sqrt{4/5}$	$-\sqrt{1/5}$		$\sqrt{1/20}$		$-\sqrt{9/10}$	$\sqrt{1/20}$					
(41)3	1						-1					
(22)0			1		$-\sqrt{5/3}$			$-2/3$				
(22)1		$\sqrt{5/3}$	$-2/3$		$\sqrt{5/6}$	$-\sqrt{5/18}$		$-2/3$	$\sqrt{5/6}$			
(22)2		1				$-\sqrt{1/18}$	$-1/2$		$-5/6$			
(30)1		1			1/6	$\sqrt{2/3}$				$-\sqrt{2/3}$	$\sqrt{1/12}$	
(30)2		1					1/2				$-\sqrt{3}/2$	
(03)1			1					$-2/3$	$-\sqrt{5}/3$			
(11)0			1					3/8		$-\sqrt{15/32}$		5/8
(11)1			1					$-1/24$	$\sqrt{5}/6$	$-\sqrt{5/96}$	$-\sqrt{5/12}$	$-5/8$

TABLE II. (*Continued*)

$q^6 \to q^5$	$(50)\frac{3}{2}$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(31)\frac{5}{2}$	[41] $(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$
[42] (60)1	1								
(41)0		1							
(41)1	1/2	−1/2	$\sqrt{2}/2$						
(41)2	$\sqrt{9/20}$		$\sqrt{1/10}$	$\sqrt{9/20}$					
(22)1			$-\sqrt{8/13}$		$\sqrt{5/13}$				
(22)1		$\sqrt{13/6}$	$\sqrt{25/234}$		$\sqrt{20/117}$	$\sqrt{13}/6$			
(22)2			$\sqrt{2}/2$	1/2		−1/2			
(22)3				1					
(30)0		$\sqrt{2/5}$					$\sqrt{3/5}$		
(30)1		$\sqrt{9/20}$					$\sqrt{2/15}$	$\sqrt{5/12}$	
(30)2			$\sqrt{2/5}$	$-\sqrt{9/20}$				$-\sqrt{3/20}$	
(03)0					1				
(03)2						1			
(11)0					5/8		$\sqrt{15/32}$		3/8
(11)1						$-\sqrt{9/20}$	$-\sqrt{8/15}$	$-\sqrt{1/60}$	
(11)1					5/8	$-\sqrt{1/20}$	$\sqrt{3/160}$	$\sqrt{3/20}$	−5/8
(11)2						1/2		$\sqrt{3}/2$	
(00)1									1

TABLE II. (*Continued*)

$q^6 \to q^5$ [311]	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(20)\frac{5}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[411] (41)1	$\sqrt{8}/3$	$-1/3$								
(41)2		1								
(22)0	2/3		$-\sqrt{5}/3$							
(22)1	$\sqrt{8}/9$	5/9	$\sqrt{40}/9$	$\sqrt{8}/9$						
(22)2		$-1/3$		$\sqrt{8}/3$						
(30)0	$-\sqrt{4/15}$				$-\sqrt{8/15}$	$-\sqrt{1/5}$				
(30)1	$-\sqrt{50/423}$	$\sqrt{16/423}$			$\sqrt{25/47}$	$-\sqrt{200/1269}$	$\sqrt{196/1269}$			
(30)1	$-\sqrt{32/2115}$	$-\sqrt{125/423}$			$\sqrt{16/235}$	$\sqrt{338/705}$	$\sqrt{20/141}$			
(30)2		$\sqrt{1/15}$					$\sqrt{4/5}$	$-\sqrt{2/15}$		
(30)3								1		
(03)1			$-\sqrt{5}/3$	2/3						
(11)0			$-\sqrt{5/24}$		$-\sqrt{1/12}$	$\sqrt{1/2}$			$-\sqrt{5/24}$	
(11)1			$-\sqrt{5/252}$	$-\sqrt{289/1008}$	$\sqrt{1/14}$	$-\sqrt{16/189}$	$-\sqrt{25/1512}$		$-\sqrt{125/252}$	$\sqrt{25/1008}$
(11)1			$\sqrt{25/504}$	$-\sqrt{5/126}$	$-\sqrt{5/28}$	$-\sqrt{5/42}$	$\sqrt{5/21}$		$-\sqrt{1/56}$	$-\sqrt{5/14}$
(11)2				$-\sqrt{1/48}$			$\sqrt{1/8}$	$\sqrt{1/3}$		$\sqrt{25/48}$
(00)0									-1	

TABLE II. *(Continued)*

$q^6 \to q^5$ [41]	$(50)\frac{3}{2}$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(31)\frac{5}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$
[411] (41)1	$\sqrt{1/2}$	$-\sqrt{1/18}$	$-2/3$						
(41)2	$\sqrt{1/2}$			$-\sqrt{1/2}$					
(22)0		$2/3$			$-\sqrt{5}/3$				
(22)1		$\sqrt{1/2}$				$-\sqrt{1/2}$			
(22)2			$2/3$	$-\sqrt{1/2}$		$\sqrt{1/18}$			
(30)0		$\sqrt{3/5}$					$-\sqrt{2/5}$		
(30)1			$-\sqrt{36/47}$				$-\sqrt{25/141}$	$\sqrt{8/141}$	
(30)1		$\sqrt{47/90}$	$-\sqrt{5/423}$				$-\sqrt{16/705}$	$-\sqrt{125/282}$	
(30)2			$\sqrt{3/5}$	$\sqrt{3/10}$				$\sqrt{1/10}$	
(30)3				1					
(03)1					$\sqrt{5}/3$	$-2/3$			
(11)0					$\sqrt{15/32}$		$-1/4$		$-\sqrt{15/32}$
(11)1						$-\sqrt{9/28}$	$\sqrt{8/21}$	$-\sqrt{25/84}$	
(11)1					$\sqrt{175/288}$	$\sqrt{5/126}$	$-\sqrt{5/336}$	$-\sqrt{5/42}$	$\sqrt{7/32}$
(11)2						$\sqrt{3}/2$		$-1/2$	
(00)0									1

TABLE II. *(Continued)*

$q^6 \to q^5$	$(50)\frac{1}{2}$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	[32] $(12)\frac{5}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[42] (60)1	1									
(41)0	3/5	4/5								
(41)1	−2/5	4/5	$-\sqrt{1/5}$							
(41)2			1							
(22)1		$\sqrt{4/13}$		$-\sqrt{5/13}$	$\sqrt{4/13}$					
(22)1		$\sqrt{16/117}$	$\sqrt{13/45}$	$\sqrt{256/585}$	$\sqrt{16/117}$					
(22)2			$-\sqrt{1/5}$		4/5	−2/5				
(22)3						1				
(30)0		$-\sqrt{2/5}$					$-\sqrt{3/5}$			
(30)1			−3/5				$\sqrt{8/15}$	$\sqrt{8/75}$		
(30)2			$\sqrt{1/25}$					$\sqrt{24/25}$		
(03)0				1						
(03)2					4/5	3/5				
(11)0				−1/2			$\sqrt{3/10}$		$-\sqrt{9/20}$	
(11)1				3/10	$\sqrt{9/80}$		$\sqrt{1/30}$	$\sqrt{121/600}$	$-\sqrt{9/20}$	$\sqrt{9/80}$
(11)1				1/10	$-\sqrt{1/5}$		$-\sqrt{3/10}$	$\sqrt{6}/5$	$-\sqrt{1/20}$	$-\sqrt{1/5}$
(11)2					$-\sqrt{1/400}$	−3/5		$\sqrt{3/40}$		3/4
(00)1									$-\sqrt{1/5}$	$-\sqrt{4/5}$

TABLE II. *(Continued)*

$q^6 \to q^5$	$(50)\frac{1}{2}$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	[32] $(12)\frac{5}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[33] (60)0	1									
(41)1	$\sqrt{1/5}$	$\sqrt{16/45}$	$\sqrt{2/3}$							
(22)0		2/3		$\sqrt{5}/3$						
(22)2			2/3		$\sqrt{16/45}$	$\sqrt{1/5}$				
(30)1		$\sqrt{2/9}$	$-\sqrt{8/45}$					$-\sqrt{1/3}$	$\sqrt{4/15}$	
(03)1				$\sqrt{5}/3$	2/3					
(03)3						1				
(11)1				$\sqrt{5}/6$	$-5/12$		$\sqrt{1/6}$	$\sqrt{5/24}$	1/2	1/4
(11)2					$\sqrt{9/80}$	$-\sqrt{1/5}$		$\sqrt{3/8}$		$-\sqrt{5}/4$
(00)0									1	

TABLE II. (*Continued*)

[32]

$q^6 \to q^5$	$(50)\frac{1}{2}$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(12)\frac{5}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[321] (41)0	4/5	−3/5								
(41)1	4/5	1/15	$-\sqrt{16/45}$							
(22)0		$\sqrt{5}/3$		−2/3						
(22)1			4/5	−2/5	$-\sqrt{1/5}$					
(22)1		$\sqrt{5}/3$	−4/15	2/15	$-\sqrt{16/45}$					
(22)2			$\sqrt{16/45}$		−1/15	−4/5				
(30)0		$\sqrt{3/5}$					$-\sqrt{2/5}$			
(30)1			$\sqrt{72/175}$				$\sqrt{4/105}$	$\sqrt{289/525}$		
(30)1		$\sqrt{7/9}$	$\sqrt{16/315}$				$\sqrt{2/21}$	$-\sqrt{8/105}$		
(30)2			$\sqrt{24/25}$					−1/5		
(03)1				2/3	$-\sqrt{5}/3$					
(03)2					3/5	−4/5				
(11)0							$\sqrt{3/5}$		$\sqrt{2/5}$	
(11)0				$\sqrt{3}/2$			$\sqrt{1/10}$		$-\sqrt{3/20}$	
(11)1					$-\sqrt{549/1096}$		$\sqrt{676/25071}$	$-\sqrt{305/1644}$	$-\sqrt{1800/8357}$	$\sqrt{4761/66856}$
(11)1							$\sqrt{27/61}$		$-\sqrt{2/61}$	$-\sqrt{32/61}$
(11)1				$\sqrt{137/180}$	$\sqrt{16/1233}$		$-\sqrt{25/822}$	$-\sqrt{338/2055}$	$\sqrt{1/548}$	$-\sqrt{4/137}$
(11)2						$-\sqrt{25/59}$		$-\sqrt{30/59}$		$-\sqrt{4/59}$
(11)2					$\sqrt{177/200}$	$\sqrt{24/1475}$		$-\sqrt{49/1180}$		$\sqrt{27/472}$
(11)3						1				
(00)1									$\sqrt{4/5}$	$-\sqrt{1/5}$
(00)2										1

TABLE II. (*Continued*)

$q^n \to q^s$	$(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	[311] $(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(20)\frac{5}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[321] (41)0	-1									
(41)1	$-1/3$	$-\sqrt{8/3}$								
(22)0	$-\sqrt{5}/3$		$-2/3$							
(22)1	$-\sqrt{256/405}$	$-\sqrt{8/405}$	$2/9$	$\sqrt{121/405}$						
(22)1	$-\sqrt{1/45}$	$-\sqrt{8/45}$	$2/3$	$-\sqrt{16/45}$						
(22)2		$-\sqrt{8/3}$		$-1/3$						
(30)0	$\sqrt{1/15}$				$\sqrt{2/15}$	$-\sqrt{4/5}$				
(30)1	$\sqrt{128/315}$	$-\sqrt{20/63}$			$\sqrt{4/35}$	$-\sqrt{128/945}$	$-\sqrt{5/189}$			
(30)1	$\sqrt{1/63}$	$\sqrt{8/63}$			$\sqrt{2/7}$	$\sqrt{4/21}$	$-\sqrt{8/21}$			
(30)2		$\sqrt{4/15}$					$-\sqrt{1/5}$	$-\sqrt{8/15}$		
(03)1			$-2/3$	$-\sqrt{5}/3$						
(03)2				-1						
(11)0			$\sqrt{1/2}$						$-\sqrt{1/2}$	
(11)0			$-\sqrt{1/12}$		$\sqrt{5/6}$				$-\sqrt{1/12}$	
(11)1			$-\sqrt{1690/75213}$	$\sqrt{1525/9864}$	$-\sqrt{3600/8357}$	$\sqrt{9800/225639}$	$-\sqrt{61/14796}$		$-\sqrt{22090/75213}$	$\sqrt{30625/601704}$
(11)1			$-\sqrt{45/122}$		$-\sqrt{4/61}$	$-\sqrt{24/61}$			$\sqrt{125/1098}$	$\sqrt{32/549}$
(11)1			$\sqrt{125/4932}$	$\sqrt{169/1233}$	$\sqrt{1/274}$	$-\sqrt{64/411}$	$-\sqrt{200/411}$		$-\sqrt{5/548}$	$-\sqrt{25/137}$
(11)2				$\sqrt{25/59}$			$\sqrt{24/59}$	$-\sqrt{9/59}$		$\sqrt{1/59}$
(11)2				$\sqrt{49/1416}$			$-\sqrt{81/236}$	$-\sqrt{32/177}$		$\sqrt{625/416}$
(11)3								-1		
(00)1									$-2/3$	$-\sqrt{5/3}$
(00)2										-1

TABLE II. (*Continued*)

$q^0 \to q^s$	$(31)\frac{1}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	[221] $(01)\frac{1}{2}$	$(01)\frac{3}{2}$	$(01)\frac{5}{2}$
[321] (41)0	1							
(41)1	-1							
(22)0	$-\sqrt{1/5}$	$\sqrt{4/5}$						
(22)1		$-\sqrt{4/5}$	$\sqrt{1/5}$					
(22)1	$\sqrt{5}/3$	$\sqrt{4/45}$	$\sqrt{16/45}$					
(22)2			-1					
(30)0	$\sqrt{3/5}$			$\sqrt{2/5}$				
(30)1				$-\sqrt{20/21}$	$\sqrt{1/21}$			
(30)1	$-\sqrt{7}/5$			$\sqrt{6/175}$	$\sqrt{24/35}$			
(30)2					-1			
(03)1		$-\sqrt{4/5}$	$-\sqrt{1/5}$					
(03)2			1					
(11)0		$\sqrt{2/5}$		$\sqrt{3/5}$				
(11)0		$\sqrt{3/20}$		$-\sqrt{1/10}$		$\sqrt{3}/2$		
(11)1		$\sqrt{1800/8357}$	$-\sqrt{4761/66856}$	$-\sqrt{8836/25071}$	$\sqrt{6125/100284}$	$-\sqrt{160/8357}$	$-\sqrt{137/488}$	
(11)1		$\sqrt{2/61}$	$\sqrt{32/61}$	$\sqrt{25/183}$	$\sqrt{64/915}$	$-\sqrt{8/2745}$	$-\sqrt{128/549}$	
(11)1		$-\sqrt{1/548}$	$\sqrt{4/137}$	$-\sqrt{3/274}$	$-\sqrt{30/137}$	$-\sqrt{405/548}$		
(11)2			$\sqrt{4/59}$		$\sqrt{6/295}$		$\sqrt{1296/1475}$	$-\sqrt{49/1475}$
(11)2			$-\sqrt{27/472}$		$\sqrt{125/236}$		$\sqrt{3/472}$	$\sqrt{24/59}$
(11)3								-1
(00)1						2/3	$-\sqrt{5}/3$	
(00)2							3/5	4/5

TABLE II. (*Continued*)

$q^6 \to q^5$	[311] $(31)\frac{1}{2}$	$(31)\frac{3}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(20)\frac{5}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[3111] (22)1	$\sqrt{20}/9$	$-\sqrt{40}/9$	1/9	$\sqrt{20}/9$						
(30)0	$\sqrt{2/3}$				$-\sqrt{1/3}$					
(30)1	2/3	$\sqrt{2/3}$				$\sqrt{1/27}$	$\sqrt{8/27}$			
(30)2		$\sqrt{2/3}$						$\sqrt{1/3}$		
(03)0			1							
(11)0			$\sqrt{5/24}$		$\sqrt{1/12}$	$\sqrt{1/2}$			$\sqrt{5/24}$	
(11)1				$\sqrt{225/592}$	$\sqrt{8/37}$	$-\sqrt{3/37}$	$\sqrt{75/296}$		$-\sqrt{20/333}$	$\sqrt{49/5328}$
(11)1			$\sqrt{37/72}$	$-\sqrt{5/2664}$	$-\sqrt{5/148}$	$-\sqrt{245/1998}$	$-\sqrt{5/3996}$		$\sqrt{25/2664}$	$\sqrt{845/2664}$
(11)2				$\sqrt{25/48}$			$-\sqrt{1/8}$	$\sqrt{1/3}$		$-\sqrt{1/48}$
(00)1									$\sqrt{5}/3$	$-2/3$

$q^6 \to q^5$	[2111] $(12)\frac{1}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$
[3111] (22)1	-1				
(30)0		1			
(30)1		$-\sqrt{2/3}$	$\sqrt{1/3}$		
(30)2			-1		
(03)0	1				
(11)0	$-\sqrt{15/32}$	$\sqrt{1/16}$		$-\sqrt{15/32}$	
(11)1	$\sqrt{125/592}$	$\sqrt{49/888}$	$-\sqrt{25/444}$	$-\sqrt{3125/5328}$	$\sqrt{121/1332}$
(11)1	$\sqrt{9/1184}$	$-\sqrt{605/1776}$	$-\sqrt{40/111}$	$-\sqrt{25/1184}$	$-\sqrt{10/37}$
(11)2			1/2		$-\sqrt{3}/2$
(00)1				$-\sqrt{5}/3$	$-2/3$

TABLE II. (*Continued*)

$q^6 \to q^5$	[221] $(31)\frac{1}{2}$	$(12)\frac{1}{2}$	$(12)\frac{3}{2}$	$(20)\frac{1}{2}$	$(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$	$(01)\frac{5}{2}$
[222]								
(22)1	2/3	−1/3	−2/3					
(30)0	$\sqrt{2/5}$			$-\sqrt{3/5}$				
(03)0		1						
(11)1		1/2	−1/4	$\sqrt{1/6}$	$\sqrt{5/24}$	$-\sqrt{5/6}$	5/12	
(11)2			$\sqrt{5}/4$		$\sqrt{3/8}$		$-\sqrt{9/80}$	$-\sqrt{1/5}$
(00)1						$\sqrt{5}/3$	2/3	
(00)3								1
[2211]								
(22)0	$\sqrt{4/5}$	$\sqrt{1/5}$						
(30)1	$\sqrt{18}/5$			$\sqrt{1/75}$	$\sqrt{4/15}$			
(03)1		$\sqrt{1/5}$	$-\sqrt{4/5}$					
(11)0		$\sqrt{9/20}$		$-\sqrt{3/10}$		−1/2		
(11)1			$\sqrt{9/32}$	$-\sqrt{1/3}$	$\sqrt{5/48}$		$\sqrt{9/32}$	
(11)1		$\sqrt{1/2}$	$\sqrt{1/32}$		$-\sqrt{27/80}$	$\sqrt{1/10}$	$\sqrt{1/32}$	
(11)2			3/4		$-\sqrt{3/40}$		−1/20	3/5
(00)0						1		
(00)2							4/5	−3/5

TABLE II. (*Continued*)

$q^5 \to q^5$	$(12)\frac{1}{2}$	$(20)\frac{1}{2}$	[2111] $(20)\frac{3}{2}$	$(01)\frac{1}{2}$	$(01)\frac{3}{2}$	[11111] $(01)\frac{1}{2}$
[2211]						
(22)0	-1					
(30)1		$\sqrt{1/3}$	$\sqrt{2/3}$			
(03)1	1					
(11)0	3/8	$-\sqrt{15/32}$		$-5/8$		
(11)1	$\sqrt{45/128}$	$\sqrt{25/192}$	$-\sqrt{1/6}$	$\sqrt{45/128}$		
(11)1	$-\sqrt{5/128}$	$\sqrt{27}/8$		$-\sqrt{5/128}$	$-\sqrt{1/2}$	
(11)2			$\sqrt{3/2}$		1/2	
(00)0				-1		
(00)2					1	
[21111]						
(11)0	5/8	$\sqrt{15/32}$		$-3/8$		1
(11)1	5/8	$-\sqrt{5/96}$	$\sqrt{5/12}$	$-1/24$	$-\sqrt{5}/6$	-1
(00)1				2/3	$-\sqrt{5}/3$	1
[111111]						
(00)0						1

$$\Psi(q^n)=(n_h)^{-1/2}\sum_{(r)}\sum\left\langle\begin{matrix}(\lambda'_f\mu'_f & (10) \\ I'\ Y' & iy\end{matrix}\middle|\begin{matrix}(\lambda_f\mu_f) \\ I\ Y\end{matrix}\right\rangle\left\langle\begin{matrix}[h'_1\cdots h_6] & [1] \\ (\lambda'_c\mu'_c)S'\omega' & (10)\frac{1}{2}\end{matrix}\middle|\begin{matrix}[h_1\cdots h_6] \\ (\lambda_c\mu_c)S\omega\end{matrix}\right\rangle$$

$$\times\{\Phi(q^{n-1}[h'_1\cdots h'_6](\lambda'_c\mu'_c)S'\omega')\phi((10)\tfrac{1}{2})\}^{(\lambda_c\mu_c)S}[\chi(q^{n-1}(\lambda'_f\mu'_f)I'Y')\chi(q^{(10)iy})]^{I\,Y}_{I_z}$$

$$=\sum(n'_h/n_h)^{1/2}\left\langle\begin{matrix}(\lambda'_f\mu'_f) & (10) \\ I'\ Y' & iy\end{matrix}\middle|\begin{matrix}(\lambda_f\mu_f) \\ I\ Y\end{matrix}\right\rangle\left\langle\begin{matrix}[h'_1\cdots h'_6] & [1] \\ (\lambda'_c\mu'_c)S' & (10)\frac{1}{2}\end{matrix}\middle|\begin{matrix}[h_1\cdots h_6] \\ (\lambda_c\mu_c)S\omega\end{matrix}\right\rangle$$

$$\times\{\Psi(q^{n-1}(\lambda'_f\mu'_f)I'Y';\ [h'_1\cdots h'_6](\lambda'_c\mu'_c)S'\omega')\psi(q(10)\tfrac{1}{2})\}^{(\lambda_f\mu_f)(\lambda_c\mu_c)S}_{I\ I_z\ Y} \tag{19}$$

Equation (19) expresses the desired separation of ψ into a series of antisymmetric wavefunctions of $n-1$ quarks and a single-quark function.

It remains to affix the phases of the SU(6) Wigner coefficients subject to the condition that $\phi([h])$ transform contragradiently with respect to $\chi(\lambda_f\mu_f)$. The ambiguity in phase arises because there are, in general, several $[f']$ of $n-1$ quarks to which a single quark may be added to obtain the representation $[f]$ of n quarks. For given $[f^{(1)}]$, $[f^{(2)}]=[1]$ and $[f](\lambda\mu)S\omega$ in the Wigner coefficient of Eq. (9), the relative phases of coefficients with different $(\lambda_1\mu_1)S_1\omega_1$ are uniquely determined by the requirement that it be an eigenvector of the matrix $\langle P\rangle$, Eq. (13). An over-all phase of each eigenvector is undetermined.

A simple example will make this more clear. The SU(6) representation [21] is important since it contains a color singlet, and the $SU(3)_f$ representation conjugate to [21] is (11), or the octet of baryons. The representation [21] may be obtained by adding a quark to either [2] or to [11]. The relevant Wigner coefficients are derived by diagonalizing two *different* matrices, and hence one has no information on the relative phase of the coefficients

$$\left\langle\begin{matrix}[2] & [1] \\ (\lambda'\mu')S' & (10)\frac{1}{2}\end{matrix}\middle|\begin{matrix}[21] \\ (\lambda\mu)S\end{matrix}\right\rangle \quad\text{and}$$

$$\left\langle\begin{matrix}[11] & [1] \\ (\lambda'\mu')S' & (10)\frac{1}{2}\end{matrix}\middle|\begin{matrix}[21] \\ (\lambda\mu)S\end{matrix}\right\rangle.$$

The *relative* phase of these two coefficients may be determined by the requirement that [21] transform in a contragradient fashion to the $SU(3)_f$ representation (11).

The transformation properties of the SU(3) Wigner coefficients may be determined by the symmetry relations of

Ref. 13. Under particle permutation, particles in the same row of the SU(3) Young tableaux are symmetric; those in the same column are antisymmetric. The representations of SU(6) must be opposite. Hence,

$$P_{n-1,n}\phi([h_1\cdots h_6](r))=-\phi([h](r))$$

or

$$P_{n-1,n}\phi([h_1\cdots h_6](r))=+\phi([h](r))$$

if n and $n-1$ are in the same row or column, respectively. If n and $n-1$ are neither in the same row nor column

$$P_{n-1,n}\phi([h](r))=-(1/a)\phi([h](r)) -(1-1/a^2)^{1/2}\phi([h](r')), \tag{20}$$

where (r') is the Yamanouchi symbol obtained by interchanging n and $n-1$, and a is the "axial distance," or number of boxes in the Young tableux $[h]$ between n and $n-1$.

If (r) is not identical with (r'), then removal of the n'th quark results in two different $[h']$, and Eq. (20) may be used in conjunction with the recurrence relation

$$\begin{aligned}&\left\langle \begin{matrix}[f'] & [1] \\ (\lambda'\mu')S'\omega' & (10)\tfrac{1}{2}\end{matrix}\middle|\begin{matrix}[f] \\ (\lambda\mu)S\omega\end{matrix}\right\rangle \\ &\times\langle[f](r)|P_{n-1,n}|[f'](r')\rangle \\ &=\sum_{(\lambda_1\mu_1)S_1\omega_1}\left\langle \begin{matrix}[f_1] & [1] \\ (\lambda_1\mu_1)S_1\omega_1 & (10)\tfrac{1}{2}\end{matrix}\middle|\begin{matrix}[f] \\ (\lambda\mu)S\omega\end{matrix}\right\rangle \\ &\times\sum_{(\lambda''\mu'')S''\omega''}\left\langle \begin{matrix}[f''] & [1] \\ (\lambda''\mu'')S''\omega'' & (10)\tfrac{1}{2}\end{matrix}\middle|\begin{matrix}[f_1] \\ ((\lambda_1\mu_1)S_1\omega_1\end{matrix}\right\rangle \\ &\times\left\langle \begin{matrix}[f'] & [f] \\ (\lambda''\mu'')S''\omega'' & (10)\tfrac{1}{2}\end{matrix}\middle|\begin{matrix}[f'] \\ (\lambda'\mu')S'\omega'\end{matrix}\right\rangle \\ &\times U(\tfrac{1}{2}S''S\tfrac{1}{2};S'S_1)(-)^{S'+S_1+S''+S} \\ &\times(-)^{\lambda''+\lambda_1+\lambda'+\lambda+\mu_1+\mu'+\mu+\mu''} \\ &\times U[(10)(\lambda''\mu'')(\lambda\mu)(10);(\lambda'\mu')(\lambda_1\mu_1)]\end{aligned} \tag{21}$$

to determine the relative phase between the representations $[h^{(1)}]$ and $[h^{(2)}]$ of $n-1$ quarks. An over-all phase remains, and this was fixed in the following (arbitrary) manner. The representations $[h_1\cdots h_6]$ were arranged in order of decreasing value of $([h_i])$, Eq. (12). Similarly, the $(\lambda\mu)$ were order by decreasing value of the SU(3) Casimir operator; the values of S were, however, by increasing value. For a given $[h](\lambda\mu)S\omega$ the first nonzero coefficient coupling a quark to $[h'](\lambda'\mu')S'\omega'$ was taken to be positive. The phases of all other coefficients leading to $[h](\lambda\mu)S\omega$ are now determined.

This prescription has one unfortunate property. The representations $[h_1\cdots h_6]$ and $[h_1+1\ h_2+1\cdots h_6+1]$ are equivalent under transformations of SU(6). Hence SU(6) Wigner coefficients connecting $[h_1+1\cdots h_6+1]$ to $[h'_1+1\cdots h'_6+1]$ should be identical to those involving the SU(6) equivalent representations $[h_1\cdots h_6]$ and $[h'_1\cdots h'_6]$. Using the above phase convention, the coefficients, although identical in magnitude (assuming no multiplicity), in general differ, by a phase. The only disadvantage apart from esthetics is that this requires the tabulation of a few additional numbers.

In the actual evaluation of the Wigner coefficients, the labels of the subgroups of SU(3) ⊗ SU(2) never enter, but they must be specified in any physical applications. There are several equivalent ways to specify the three sublabels of representations of SU(3). The more familiar method uses hypercharge, isospin, and its z projection, i.e., the labels of a U(1) subgroup (hypercharge) and an SU(2) subgroup (isospin) and its subgroup label, I_z. These are the canonical subgroups of SU(3) and, hence, there is no multiplicity. The scheme used in Eq. (16) to label the subgroups of $SU(3)_c$ is in complete analogy. The quantum numbers used were ϵ, Λ, and ν with Λ, ν analogous to I, I_z and ϵ analogous to hypercharge. The allowed values of ϵ, Λ, and ν for an SU(3) $(\lambda\mu)$ are

$$\begin{aligned}&\epsilon=p+q-\tfrac{1}{3}(2\lambda+\mu), \\ &\Lambda=\tfrac{1}{2}(\mu+p-q), \\ &\nu=r-\Lambda\end{aligned} \tag{22}$$

with the integers p, q, and r restricted by the conditions

$$\begin{aligned}&0\leqslant p\leqslant\lambda, \\ &0\leqslant q\leqslant\mu, \\ &0\leqslant r\leqslant\mu+p-q.\end{aligned} \tag{23}$$

An alternate scheme for $SU(3)_c$ is to define the Cartesian quantum numbers n_1, n_2, and n_3:

$$\begin{aligned}&n_1=\tfrac{1}{3}(N-\lambda)+r-\tfrac{2}{3}\mu+q, \\ &n_2=\tfrac{1}{3}(N-\lambda)-r+\tfrac{2}{3}\mu+p, \\ &n_3=\tfrac{1}{3}(N+2\lambda+\mu)-p-q,\end{aligned} \tag{24}$$

with N the total number of quarks. The n_i specify the number of quarks of each color. It is immediately clear that for a color singlet, $(\lambda\mu)=(00)$, the number of quarks for each color is $1/3N$.

5. AN EXAMPLE

In this section a brief example of the application of the SU(6) Wigner coefficients will be given. A possible excited state of the nucleon may be constructed from four quarks and an antiquark, $q^4\bar{q}$, Among the many possible SU(6) and $SU(3)_c$ representations of q^4 configuration is

$$\left|\begin{matrix}q^4 & [31] & (10)_f & I\ Y\ I_z \\ & (10)_c & S_{q=0} & n_1n_2n_3\end{matrix}\right\rangle. \tag{25}$$

It is essential that the $SU(3)_c$ representation of the four-quark state be $(10)_c$ as the $\bar{q}$ state has representation $(01)_c$ and the total state must have representation $(00)_c$. The choice of the $SU(3)_f$ representation $(10)_f$ is dictated by the requirement that it be conjugate to [31].

To calculate the decay probability of a $q^4\bar{q}$ state into a baryon and a meson, one decouples a single quark from the

four quark state of Eq. (25) by using the SU(6) Wigner coefficients and then recouples this quark with an anti-quark to form a meson. This latter step involves only Racah coefficients and will not be dealt with here.

Using the coefficients from the table, one has

$$\left|q^4 \begin{matrix}[31] & (10)_f & IY & I_z \\ (10)_c & 0 & \epsilon\Lambda & \nu\end{matrix}\right\rangle$$

$$=\sum_{f'}\left(\frac{n_{f'}}{n_{[31]}}\right)^{1/2}\left\langle \begin{matrix}[f'] & & [1] & \\ (\lambda'\mu')_c & S' & \otimes & (10)\tfrac{1}{2}\end{matrix}\middle|[31]\right\rangle$$

$$\times\left\langle \begin{matrix}(\lambda'\mu') & (10) & \\ \epsilon'\Lambda' & \epsilon_1\Lambda_1 & \end{matrix}\middle|\begin{matrix}(10) \\ \epsilon\Lambda\end{matrix}\right\rangle\left\langle \begin{matrix}(\bar{\lambda}\bar{\mu})_f & (10)_f & \\ \bar{I}\,\bar{Y} & iy & \end{matrix}\middle|\begin{matrix}(10)_f \\ IY\end{matrix}\right\rangle$$

$$\times\left[\left|q^3 \begin{matrix}[f'] & (\bar{\lambda}\bar{\mu})_f \\ (\lambda'\mu')_c & S'\end{matrix}\right\rangle\left|q \begin{matrix}[1] & (10)_f \\ (10)_c & \tfrac{1}{2}\end{matrix}\right\rangle\right]^{IY\Lambda\epsilon}_{I_z\nu}. \tag{26}$$

The physics requires $(\lambda'\mu')_c$ to be a color singlet, (00). The only SU(6) representation of three quarks which contains a color singlet and will connect with [31] is [21]. The $SU(3)_f$ representation is then $(11)_f$, or an octet. Hence, one has immediately the selection rule that the state, Eq. (25), will not decay into the decuplet plus a quark. Equation (26) becomes

$$\sqrt{\frac{2}{3}}\sqrt{\tfrac{1}{2}}\left\langle \begin{matrix}(11)_f & (10) & \\ \bar{I}\,\bar{Y} & iy & \end{matrix}\middle|\begin{matrix}(10)_f \\ IY\end{matrix}\right\rangle$$

$$\times\left[\left|q^3 \begin{matrix}[21] & (11)_f \\ (00)_c & \tfrac{1}{2}\end{matrix}\right\rangle\left|q \begin{matrix}[1] & (10)_f \\ (10)_c & \tfrac{1}{2}\end{matrix}\right\rangle\right]^{IY\,\epsilon\Lambda}_{I_z\nu}$$

$$+\text{terms with } (\lambda'\mu')_c\neq(00)_c$$

The SU(3) Wigner coefficients which determine the decay rates to the various members of the baryon octet are easily evaluated.[14,20]

Although the above example is straightforward, more involved problems may be performed in an identical manner with the use of the SU(6) Wigner coefficients tabulated here. Similarly, calculations involving several quarks coupling to several antiquarks may also be done by constructing several particle fractional parentage coefficients from the ones tabulated here.[15]

APPENDIX

Jaffe has obtained an equation with which to evaluate the expectation value of the Casimir operator $C_2(6)$ of SU(6). It requires a knowledge of the reduction of SU(6) into its subgroups SU(3) ⊗ SU(2), and is a generalization of the technique used by Frobenius[21] for the symmetric group. The expression obtained by Jaffe is unsatisfactory in many cases as it involves a summation over all the representations of SU(3) ⊗ SU(2), of which there may be many, and which may not be known, although from the present work the reduction is complete for the cases of nine or fewer quarks.

We derive here in the standard manner an expression for the quadratic Casimir operator of SU(n). In terms of the n^2-1 generators of SU(n), the Casimir operator is

$$C_2(n)=\sum \bar{C}_{\alpha\beta}\bar{C}_{\beta\alpha}, \tag{A1}$$

where $\bar{C}_{\alpha\beta}$ are the traceless generators of SU(n):

$$\bar{C}_{\alpha\beta}=C_{\alpha\beta}-\frac{1}{n}\,\delta_{\alpha\beta}\mathrm{Tr}(C_{\alpha\alpha}). \tag{A2}$$

The $\bar{C}_{\alpha\beta}$ may be divided into three categories:

raising $\alpha<\beta$,

lowering $\alpha>\beta$,

weight $\alpha=\beta$.

Acting on a state of highest weight, the raising operators give zero, and the weight operators

$$\bar{C}_{\alpha\alpha}|\mathrm{HW}\rangle=\bar{C}_{\alpha\alpha}|[f_1\cdots f_n]\rangle=f_\alpha|[f_1\cdots f_n]\rangle, \tag{A3}$$

where the HW indicates a state of highest weight. Hence,

$$C_2(n)|\mathrm{HW}\rangle=\left\{\sum_\alpha(\bar{C}_{\alpha\alpha})^2+\sum_{\alpha<\beta}C_{\alpha\beta}C_{\beta\alpha}\right\}|\mathrm{HW}\rangle$$

$$=\left\{\sum_\alpha(\bar{C}_{\alpha\alpha})^2+\sum_{\alpha<\beta}(C_{\alpha\alpha}-C_{\beta\beta})\right\}|\mathrm{HW}\rangle \tag{A4}$$

by virtue of the commutation relations. Thus, we obtain

$$C_2(n)|[f_1\cdots f_n]\rangle=\left\{\sum_\alpha f_\alpha^2-\frac{1}{n}(\sum f_\alpha)^2\right\}$$

$$+\sum_{\alpha=1}^{[n/2]}(n+1-2\alpha)(f_\alpha-f_{n+1-\alpha})\Big|\rangle, \tag{A5}$$

where $[n/2]$ is defined to be the integral part of $n/2$.

Using Eq. (A5), one obtains immediately:

SU(2): $S=\frac{1}{2}(f_1-f_2)$, $\quad C_2(2)=2S(S+1)$;

SU(3): $\lambda=f_1-f_2$,

$\mu=f_2-f_3$,

$C_2(3)=\frac{2}{3}(\lambda^2+\mu^2+\lambda\mu+3\lambda+3\mu)$;

SU(6): $C_2(6)=\sum_\alpha f_\alpha^2-\frac{1}{6}(\sum f_\alpha)^2$

$+5(f_1-f_6)+3(f_2-f_5)+f_3-f_4$.

To obtain Jaffe's value for $C_2(6)$, one must multiply the above expression by 4.

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Foundation of geometrical optics in general relativistic dispersive media

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Geometrical optics in dispersive media is rigorously derived from Maxwell's equations by employing the two-timing method. An effect analogous to Faraday rotation is found for the polarization plane of the wave, with the vorticity of the medium taking the place of the magnetic field.

INTRODUCTION

Geometrical optics describes radiation propagating through a medium in terms of rays along which the energy-flux propagates (at least in isotropic media).[1] In its essence geometrical optics consists of three basic assumptions:

(i) The existence of a congruence of curves called "rays."

(ii) A conservation equation for the fields square amplitude along the rays.

(iii) A transport law for the "polarization vector" of the field along the rays.

In the case of radiation propagating in vacuo the transition from Maxwell's equations to geometrical optics is easily achieved with the help of an expansion in terms of asymptotic waves.[2] A similar result can be derived in the case of a purely refractive (nondispersive) medium by using the so-called "optical metric."[2,3]

In the case of dispersive media no such rigorous transition was available. An early attempt to overcome this difficulty is due to Madore.[4] However Madore's approach is not based upon a systematic approximation procedure, but is heavily dependent on a definition of plane wave in a curved space which seems "ad hoc." The problem was recently considered by the authors in the case of an electromagnetic wave propagating in a simple dispersive medium.[5] In this paper we extend our previous results and treat in a detailed and comprehensive way a more general case.

In Sec. 2 we explain the basic mathematical technique which is essentially the two-timing method. Then we discuss in detail the case of a plasma that can be treated as a perfect fluid (a case which is frequent in astrophysics). Finally we solve the oscillatory initial value problem for the fluid coupled to the electromagnetic field. This final result shows the mathematical reliability of the method.

In Sec. 3 we turn our attention to the physical interpretation of the results. First of all we show how to derive the laws of geometrical optics from the transport equations for the zeroth order fields. A new result appears in connection with the transport equation for the polarization vector. It is found that the polarization plane rotates by an amount dependent on the fluid's vorticity, an effect which could be important in astrophysical situations. Also we compare this result with what is known in the case of purely refractive media.

Finally we show how the standard Faraday rotation can be easily incorporated in this formalism. We note that the topics treated in the present paper are not of a purely academic interest, but have some bearing on astrophysics.

In fact the propagation of radiation in relativistic dispersive media occurs quite naturally when dealing with radiative transfer in accretion discs around black holes.[6]

1. NOTATION AND CONVENTION

Space–time $\mathcal{M}$ is assumed to be a four-dimensional pseudo-Riemannian manifold with metric signature $+2$. Latin indices $a,b,\cdots$, etc. run from 0 to 3. ∇_a, d and δ denote the operators of covariant derivative, exterior derivative, and exterior coderivative, respectively. A * means taking the adjoint, e.g., ${}^*B_a=(1/3!)\eta_{abcd}B^{bcd}$ where η_{abcd} is the volume element 4-form.

2. GENERAL FORMALISM

In this paper our considerations are purely local. By introducing the electromagnetic field 2-form F, $F=F_{ab}\times dx^a\wedge dx^b$, Maxwell's equations in the presence of charges and currents write

$$dF=0, \tag{1}$$

$$d{}^*F=j, \tag{2}$$

where j is a 3-form representing the electromagnetic 4-current. Equation (2) can also be written in the form

$$\delta F=\gamma, \tag{2'}$$

where $\gamma={}^{*-1}j$.

Now we construct a suitable model for the medium. We make the following assumptions: (i) the medium consists of two noninteracting components, the ion and the electron component; (ii) the energy-momentum for the electron com-

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ponent is that of a perfect fluid, i.e.,

$$T_{ab}=\mu u_a u_b+p(g_{ab}+u_a u_b), \tag{3}$$

where μ, u^a, and p are the energy density, 4-velocity, and pressure of the electrons; (iii) because of the larger proton mass the ionic component remains unperturbed in the presence of the wave.

From assumption (i) it follows that the electron and ion number are separately conserved.

Assumption (ii) means that we neglect any dissipative effects in the electron fluid. In particular the heat conduction term is omitted in the energy–momentum tensor. γ is given by

$$\gamma^a=4\pi e(nu^a-n_i u_i^a), \tag{4}$$

where e is the electron charge, n_i, u_i^a are the ion number density and 4-velocity, and n is the electron number density.

The final equations are (1) and (2) with γ defined by (4), together with the equation of motion for the electron component,

$$\nabla_a T^{ab}=enF^{bc}u_c \tag{5}$$

where the electron number conservation equation,

$$\nabla_a(nu^a)=0. \tag{6}$$

To these we must add the normalization condition on the 4-velocity u^a,

$$u_a u^a=-1. \tag{7}$$

Now we linearize equations (1)–(7) around an unperturbed state with $F=0$. In the next section we show how a background electromagnetic field can be incorporated in this formalism. If we denote by $\hat{F}$, $\hat{n}$, $\hat{u}$, $\hat{\mu}$, and $\hat{p}$ the perturbations to the electromagnetic field, number density, 4-velocity, energy density and pressure, the linearized equations give

$$d\hat{F}=0, \tag{8}$$

$$\delta\hat{F}=4\pi\hat{\gamma},\quad \hat{\gamma}^a=e[n\hat{u}^a+\hat{n}u^a], \tag{9}$$

$$\nabla_a\hat{T}^{ab}+en\hat{F}^{ab}u_a=0, \tag{10}$$

$$\delta\hat{\gamma}=0, \tag{11}$$

$$u_a\hat{u}^a=0. \tag{12}$$

Now we look for solutions of Eqs. (8)–(12) in the form of asymptotic waves. We adopt the so-called two-timing method which has been amply expounded in the literature[7] and used in relativity by MacCallum and Taub.[8]

This method consists of assuming that, in a given coordinate system (x^a), the equantities $\hat{F}^{ab}$, $\hat{n}$, $\hat{u}^b$, $\hat{\mu}$, $\hat{p}$ are of the following form: $\hat{F}^{ab}=\hat{F}^{ab}(\epsilon x^c,(1/\epsilon)\Theta(\epsilon x^c))$, $\hat{n}=\hat{n}(\epsilon x^c,(1/\epsilon)\Theta(\epsilon x^c))$, etc. The (unperturbed) background fields g_{ab}, n, u^a, p, μ are assumed to vary on the slow scale, i.e., their dependence on the spacetime coordinates (x^a) and the scale ratio ϵ is assumed to be of the form $g_{ab}(x^c,\epsilon)=G_{ab}(\epsilon x^c)$, $n(x^c,\epsilon)=N(\epsilon x^a)$, $u^a(x^b,\epsilon)=U^a(\epsilon x^b)$, $\mu(x,\epsilon)=M(\epsilon x)$, $p(x,\epsilon)=P(\epsilon x)$, where G_{ab}, M, N, P, U^a are functions $O(1)$ of the respective arguments.

It is convenient to use the auxiliary variables $X^a=\epsilon x^a$, $\theta=(1/\epsilon)\Theta(\epsilon x^a)$. For fixed $\epsilon>0$ the X^a can be interpreted as "slow" spacetime coordinates. The small parameter ϵ then measures the ratio of the fast length scale to the slow one. If we write $f=f(X^a,\theta)$ and define

$$f_{,a}\equiv\frac{\partial f}{\partial x^a},\quad \dot{f}\equiv\frac{\partial f}{\partial\theta},$$

then

$$\frac{\partial f}{\partial x^a}=\epsilon f_{,a}+l_a\dot{f},$$

where

$$l_a\equiv\frac{\partial\theta}{\partial x^a}=\frac{\partial\Theta}{\partial x^a}=\Theta_{,a}$$

is the normal to the wavefront $\theta=$const.

For the connection coefficients $\Gamma^a{}_{bc}(x^d,\epsilon)$, with respect to the coordinate system (X^a) we have

$$\Gamma^a{}_{bc}=\epsilon\hat{\Gamma}^a{}_{bc},$$

$$\hat{\Gamma}^a{}_{bc}=\tfrac{1}{2}G^{ad}(G_{db,c}+G_{dc,b}-G_{bc,d}),$$

whence $\Gamma^a{}_{bc}=O(\epsilon)$. Henceforth a semicolon will indicate the covariant derivative computed with respect to the slow variables X^a, i.e.,

$$A_{b;a}\equiv A_{b,a}-\hat{\Gamma}^c{}_{ba}A_c.$$

Also it is convenient to define the exterior derivative operator $\hat{d}$ relative to the slow variables X^a, i.e.,

$$\hat{d}\omega=\omega_{i_1\cdots i_n;a}\,dX^a\wedge dX^{i_1}\wedge\cdots\wedge dX^{i_n},$$

$$\omega=\omega_{i_1\cdots i_n}\,dX^{i_1}\wedge\cdots\wedge dX^{i_n}.$$

Similarly let us denote by $\hat{\delta}$ the exterior coderivative operator relative to the slow variables.

Then the basic equations (8)–(11) read in terms of the slow and fast variables, with $l=d\theta$,

$$l\wedge\dot{\hat{F}}+\epsilon\hat{d}\hat{F}=0, \tag{13}$$

$$^{-1}{}^{*}(l\wedge{}^{*}\dot{\hat{F}})+\epsilon\hat{\delta}\hat{F}=4\pi\hat{\gamma}, \tag{14}$$

$$l_a\dot{\hat{T}}^{ab}+\epsilon\hat{T}^{ab}{}_{;a}+en\hat{F}^{ab}u_a=0, \tag{15}$$

$$^{-1}{}^{*}(1\wedge{}^{*}\dot{\hat{\gamma}})+\epsilon\hat{\delta}\hat{\gamma}=0. \tag{16}$$

Now we assume that the following formal asymptotic expansions hold:

$$\hat{\mu}=\sum_{q=0}^{\infty}\epsilon^q\hat{\mu}_{(q)}, \tag{17a}$$

$$\hat{n}=\sum_{q=0}^{\infty}\epsilon^q\hat{n}_{(q)}, \tag{17b}$$

$$\hat{p}=\sum_{q=0}^{\infty}\epsilon^q\hat{p}_{(q)}, \tag{17c}$$

$$\hat{u}^a=\sum_{q=0}^{\infty}\epsilon^q\hat{u}_{(q)}{}^a, \tag{17d}$$

$$\hat{F}^{ab}=\sum_{q=0}^{\infty}\epsilon^q\hat{F}_{(q)}{}^{ab}. \tag{17e}$$

Substituting into Eqs. (13)–(16) we obtain at the zeroth order:

$$l \wedge \underset{(0)}{\dot{\hat{F}}} = 0, \tag{18}$$

$$*\left(l \wedge \underset{(0)}{*\dot{\hat{F}}}\right) + 4\pi \underset{(0)}{\hat{\gamma}} = 0, \tag{19}$$

$$l_a \underset{(0)}{\dot{\hat{T}}}^{ab} + en \underset{(0)}{\hat{F}}^{ab} u_a = 0, \tag{20}$$

$$*\left(l \wedge \underset{(0)}{*\dot{\hat{\gamma}}}\right) = 0, \tag{21}$$

and for the higher orders one gets:

$$l \wedge \dot{\hat{F}}_{(q+1)} + \hat{d}\hat{F}_{(q)} = 0, \tag{22}$$

$$*(l \wedge *\dot{\hat{F}}_{(q+1)}) - \hat{\delta}\hat{F}_{(q)} + 4\pi\hat{\gamma} = 0, \tag{23}$$

$$l_a \dot{\hat{T}}_{(q+1)}{}^{ab} + \hat{T}_{(q)}{}^{ab}{}_{;a} + en\hat{F}_{(q+1)}{}^{ab} u_a = 0, \tag{24}$$

$$*(l \wedge *\dot{\hat{\gamma}}_{(q+1)}) + \hat{\delta}\hat{\gamma}_{(q)} = 0. \tag{25}$$

Now we assume the following explicit dependence on θ

$$\hat{F}_{(0)\,ab} = \Psi_{(0)\,ab} \cos\theta, \tag{26a}$$

$$\hat{F}_{(q)\,ab} = \Psi_{(q)\,ab} \cos\theta + \tilde{\Psi}_{(q)\,ab} \sin\theta, \quad q \geqslant 1 \tag{26b}$$

$$\hat{T}_{(q)\,ab} = S_{(q)\,ab} \cos\theta + \tilde{S}_{(q)\,ab} \sin\theta, \tag{26c}$$

$$\hat{u}_{(q)}{}^a = V_{(q)}{}^a \cos\theta + \tilde{V}_{(q)}{}^a \sin\theta, \tag{26d}$$

$$\hat{n}_{(q)} = N_{(q)} \cos\theta + \tilde{N}_{(q)} \sin\theta, \tag{26e}$$

$$\hat{\mu}_{(q)} = M_{(q)} \cos\theta + \tilde{M}_{(q)} \sin\theta, \tag{26f}$$

$$\hat{p}_{(q)} = P_{(q)} \cos\theta + \tilde{P}_{(q)} \sin\theta. \tag{26g}$$

Assumption (26a) corresponds to a linearly polarized wave.

Our first aim is to derive a dispersion relation from the consistency requirements for Eqs. (18)–(21). Equations (18)–(21) can be rewritten, since $*(l \wedge *\omega) = l^a \omega_a$ where ω is any form,

$$l \wedge \Psi_{(0)} = 0, \tag{28}$$

$$-l_a \Psi_{(0)}{}^{ab} + 4\pi e\,[n\tilde{V}_{(0)}{}^b + \tilde{N}_{(0)} u^b] = 0, \tag{29}$$

$$l_a \tilde{S}_{(0)}{}^{ab} + en\Psi_{(0)}{}^{ab} u_a = 0, \tag{30}$$

$$l_a S_{(0)}{}^{ab} = 0, \tag{30'}$$

$$n l_a V_{(0)}{}^a + N_{(0)} \Omega = 0, \tag{31}$$

$$n l_a \tilde{V}_{(0)}{}^a + \tilde{N}_{(0)} \Omega = 0, \tag{31'}$$

where $\Omega = u_a l^a$ is the local frequency of the wave relative to an observer at rest with the medium. Also from Eq. (12) we have

$$u_a \tilde{V}_{(0)}{}^a = 0, \quad u_a V_{(0)}{}^a = 0. \tag{32}$$

From (29') contracting with u_a we find $N_{(0)} = 0$, $V_{(0)}{}^a = 0$. From (28) we have

$$\Psi_{(0)} = l \wedge B_{(0)}, \tag{33}$$

where $B_{(0)}$ is a 1-form determined up to the transformation $B_{(0)} \to B_{(0)} + \lambda l$. We can always choose λ such that

$$B_{(0)\,a} u^a = 0 \tag{33'}$$

because one has $\Omega = l_a u^a \neq 0$ everywhere. Therefore, Eqs. (29) and (30) can be rewritten as:

$$-l^2 B_{(0)}{}^b + l^b (B_{(0)}{}^a l_a) + 4\pi e\,[n\tilde{V}_{(0)}{}^b + \tilde{N}_{(0)} u^b] = 0, \tag{34}$$

$$l_a \tilde{S}_{(0)}{}^{ab} + en\Omega B_{(0)}{}^b = 0, \tag{35}$$

where,

$$\tilde{S}_{(0)}{}^{ab} = (\mu + p)[\tilde{V}_{(0)}{}^a u^b + u^a \tilde{V}_{(0)}{}^b] + (\tilde{M}_{(0)} + \tilde{P}_{(0)}) u^a u^b + \tilde{P}_{(0)} g^{ab}.$$

Consistently with our Ansatz (ii) we assume the adiabatic law. Let $f = (\mu + p)/mn$ be the specific enthalpy, $f = (1/m)\nu$, where ν is the chemical potential. Then the adiabatic hypothesis requires

$$\hat{\mu} = mf\hat{n}, \quad \hat{p} = mnf. \tag{36}$$

At the zeroth order Eq. (36) can be written

$$\tilde{M}_{(0)} = mf\tilde{N}_{(0)}. \tag{36'}$$

By contracting (35) with u_b one rederives the standard conservation law, Eq. (31'). Then (35) can be rewritten as follows:

$$mfn\Omega\,\tilde{V}_{(0)}{}^b + P_{(0)}(\Omega u^b + l^b) + en\Omega B_{(0)}{}^b = 0 \tag{37}$$

and substituting back into (34) we obtain

$$\left[\frac{m}{e} fl^2 - 4\pi en\right]\tilde{V}_{(0)}{}^b + \left[\frac{l^2}{en}\tilde{P}_{(0)} + 4\pi e\tilde{N}_{(0)}\right] u^b - \left[\frac{m}{e} f l_a \tilde{V}_{(0)}{}^a + \frac{\Omega}{en}\tilde{P}_{(0)}\right] l^b = 0. \tag{38}$$

Contracting Eq. (38) with u_b yields:

$$(l^2 + \Omega^2)\,\tilde{P}_{(0)} + 4\pi e^2 n\tilde{N}_{(0)} + mnf\Omega(l_a \tilde{V}_{(0)}{}^a) = 0. \tag{39}$$

Now, for any reasonable equation of state we have

$$\hat{p} = K\hat{n}, \tag{40}$$

where K is some scalar function of the unperturbed state. At the zeroth order (40) reads

$$\tilde{P}_{(0)} = K\tilde{N}_{(0)}. \tag{40'}$$

From (31'), (39), and (40') it follows that in order to have nontrivial solutions for $l_a \tilde{V}_{(0)}{}^a$ and $\tilde{N}_{(0)}$,

$$K(l^2 + \Omega^2) + 4\pi e^2 n - mf\Omega^2 = 0. \tag{41}$$

Equation (41) can be written in the orthonormal Lorentz frame at a given spacetime point. Then $l^2 = -\Omega^2 + \Sigma_1^3 (l_\mu)^2$ in this frame. It follows, dividing by $\Omega \neq 0$, that

$$K\frac{\Sigma_1^3 (l_\mu)^2}{\Omega} - mf + \frac{4\pi e^2 n}{\Omega^2} = 0. \tag{41'}$$

Now we take the high frequency limit of Eq. (41'), $\Omega \to \infty$. We know that in this limit the rays are null geodesics, i.e., $\Sigma_1^3 (l_\mu)^2 = \Omega^2$. It follows that

$$K = mf \tag{42}$$

which, after substituting back into (41) yields

$$l^2 = -\frac{4\pi e^2 n}{mf}. \tag{43}$$

Again, substituting back into (38) we find

$$(8\pi e n)\,\tilde{V}_{(0)}{}^{b} = 0,$$

which yields $\tilde{V}_{(0)}{}^{b} = 0$, leading in its turn to $\tilde{N}_{(0)} = 0$. Therefore, we reached a contradiction which can only be resolved by assuming that Eqs. (31′), (39), and (40) admit only trivial solutions, i.e.,

$$l_a \tilde{V}_{(0)}{}^{a} = 0, \quad \tilde{N}_{(0)} = 0, \quad \tilde{P}_{(0)} = 0. \tag{44}$$

Finally, from (44), (38), and the requirement $\tilde{V}_{(0)}{}^{b}$ we reobtain (43) as a dispersion relation, i.e.,

$$l^2 = -\frac{4\pi e^2 n}{mf}. \tag{45}$$

Remembering that $l_a = \Theta_{,a}$, Eq. (45) is then the exact analog of the eikonal equation. Likewise, it can be solved by the method of characteristic curves. Let us define the rays

$$\frac{dX^a}{dr} = l^a = g^{ab}\Theta_{,b}. \tag{46}$$

Then one has, for the rate of variations of Θ along the rays,

$$\frac{d\Theta}{dr} = -\left(\frac{4\pi e^2}{m}\right)\frac{n}{f} \tag{47}$$

which can be solved for Θ once the initial value has been assigned on an initial hypersurface Σ transverse to the rays.

Now we are ready to derive the transport equations for the field quantities. For this we resort to Eqs. (22)–(25), which read, after having substituted (26a)–(26g):

$$-l \wedge \Psi_{(q+1)} + \hat{d}\,\hat{\Psi}_{(q)} = 0, \tag{48a}$$

$$l \wedge \tilde{\Psi}_{(q+1)} + \hat{d}\,\Psi_{(q)} = 0, \tag{48b}$$

$$-l_a \Psi_{(q+1)}{}^{ab} + \tilde{\Psi}_{(q)}{}^{ab}{}_{;a} + 4\pi e\,[n\,\tilde{V}_{(q+1)}{}^{b} + \tilde{N}_{(q+1)} u^b] = 0, \tag{49a}$$

$$l_a \tilde{\Psi}_{(q+1)}{}^{ab} + \Psi_{(q)}{}^{ab}{}_{;a} + 4\pi e\,[n\,V_{(q+1)}{}^{b} + N_{(q+1)} u^b] = 0, \tag{49b}$$

$$-l_a S_{(q+1)}{}^{ab} + \tilde{S}_{(q)}{}^{ab}{}_{;a} + en\,\tilde{\Psi}_{(q+1)}{}^{ab} u_a = 0, \tag{50a}$$

$$l_a \tilde{S}_{(q+1)}{}^{ab} + S_{(q)}{}^{ab}{}_{;a} + en\,\Psi_{(q+1)}{}^{ab} u_a = 0, \tag{50b}$$

$$-n l_a V_{(q+1)}{}^{a} - N_{(q+1)}\Omega + [n\,\tilde{V}_{(q)}{}^{a} + \tilde{N}_{(q)} u^a]_{;a} = 0, \tag{51a}$$

$$n l_a \tilde{V}_{(q+1)}{}^{a} + \tilde{N}_{(q+1)}\Omega + [n\,V_{(q)}{}^{a} + N_{(q)} u^a]_{;a} = 0. \tag{51b}$$

The solutions to Eqs. (48) can be written in the form

$$\Psi_{(q+1)} = \hat{d} A_{(q)} + l \wedge B_{(q+1)}, \tag{52a}$$

$$\tilde{\Psi}_{(q+1)} = -\hat{d} B_{(q)} + l \wedge A_{(q+1)}, \tag{52b}$$

where $A_{(q)}$ $B_{(q)}$ are 1-forms, with $A_{(0)} = 0$. We recall that

$$\Psi_{(0)} = l \wedge B_{(0)}, \quad \tilde{\Psi}_{(0)} = 0.$$

Now we prove the following proposition.

Proposition: We can always choose $A_{(q)}$, $B_{(q)}$ such that $l^a A_{(q)\,a} = l^a B_{(q)\,a} = 0$.

Proof: We proceed by induction. $A_{(0)}$ and $B_{(0)}$ verify the above condition, that is easily seen by contracting Eq. (37) with l_b. Suppose that $A_{(q)}$, $B_{(q)}$ verify $l^a A_{(q)\,a} = l^a B_{(q)\,a} = 0$. Then $A_{(q+1)}$ and $B_{(q+1)}$ are defined up to the transformations

$$A_{(q+1)} \to A_{(q+1)} + \lambda l, \quad B_{(q+1)} \to B_{(q+1)} + \lambda l.$$

Because $l^2 = g^{ab} l_a l_b \neq 0$ we can always choose λ such that

$$l^a A_{(q+1)} = l^a B_{(q+1)} = 0. \qquad \text{Q.E.D}$$

Then Eqs. (49) yield for $q \geqslant 0$

$$2DA_{(q)}{}^{b} + l^a{}_{;a} A_{(q)}{}^{b} - l^b A_{(q)}{}^{a}{}_{;a} - l^2 B_{(q+1)}{}^{b} + B_{(q-1)}{}^{b;a}{}_{;a} - B_{(q-1)}{}^{a;b}{}_{;a} + 4\pi e\,[n\,\tilde{V}_{(q+1)}{}^{b} + \tilde{N}_{(q+1)} u^b] = 0, \tag{53a}$$

$$2DB_{(q)}{}^{b} + l^a{}_{;a} B_{(q)}{}^{b} - l^b B_{(q)}{}^{a}{}_{;a} + l^2 A_{(q+1)}{}^{b} + A_{(q-1)}{}^{a;b}{}_{;a} - A_{(q-1)}{}^{b;a}{}_{;a} + 4\pi e\,[n\,V_{(q+1)}{}^{b} + N_{(q+1)} u^b] = 0, \tag{53b}$$

where $D = {}_{;a} l^a$ is the derivative along the rays and we set

$$B_{(-1)} = A_{(-1)} = 0.$$

Now we consider the zeroth order equations. The zeroth order quantities are:

$$V_{(0)}{}^{a} = 0, \tag{54a}$$

$$\tilde{V}_{(0)}{}^{a} = -\frac{e}{mf} B_{(0)}{}^{a}, \tag{54b}$$

$$N_{(0)} = \tilde{N}_{(0)} = M_{(0)} = \tilde{M}_{(0)} = 0, \tag{54c}$$

$$A_{(0)}{}^{a} = 0. \tag{54d}$$

From (50 and (51) we obtain $\tilde{V}_{(1)}, \tilde{N}_{(1)}, V_{(1)}, N_{(1)}$ in terms of $A_{(0)}, B_{(0)}, A_{(1)}, B_{(1)}$. Then, Eq. (53a) gives an identity whereas (53b) yields, after some manipulations,

$$2DB_{(0)}{}^{b} + l^a{}_{;a} B_{(0)}{}^{b} - \frac{\omega_p^2}{f\Omega} B_{(0)\,a}\,\omega^{ab} + \text{term parallel to } u^b \text{ and } l^b = 0. \tag{55}$$

By contracting Eq. (55d) with $B_{(0)}{}^{b}$ we obtain the transport equation for the square of the amplitude

$$B_{(0)}{}^{2} = B_{(0)\,b} B_{(0)}{}^{b}$$

$$DB_{(0)}{}^{2} + l^a{}_{;a} B_{(0)}{}^{2} = 0 \tag{56}$$

which is the standard amplitude-area law of geometrical optics.

Now we write $B_{(0)}{}^{b} = B_{(0)} e^b$, with $e_b e^b = 1$. e^b is the polarization unit vector of the wave. Also, at each spacetime point we introduce an orthonormal tetrad $\{u^a, \nu^a, e_{(1)}{}^{a}, e_{(2)}{}^{a}\}$, ν^a is the wave's propagation unit vector in the fluid's rest frame,

$$\nu^a = \frac{l^a + \Omega u^a}{(l^2+\Omega^2)^{1/2}}, \tag{57}$$

$e_{(1)}{}^a$ and $e_{(2)}{}^a$ are two spacelike unit vectors, orthogonal to each other and to u^a, ν^a. At each point $e_{(1)}{}^a$ and $e_{(2)}{}^a$ are defined up to an orthogonal transformation. We exploit this arbitrariness in the definition of $e_{(1)}{}^a$ and $e_{(2)}{}^a$ by choosing them to satisfy

$$e_{(2)}{}^a De_{(1)a} = 0. \tag{58}$$

Since e^a lies in the 2-plane spanned by $e_{(1)}{}^a$ and $e_{(2)}{}^a$ we write

$$e^{(a)} = \cos\Psi e_{(1)}{}^a + \sin\Psi e_{(2)}{}^a.$$

Then, contracting Eq. (55) with $e_{(1)}{}^a$ and using the condition (58) yields

$$2D\Psi + \frac{l^2}{\Omega f}\omega^{cb} e_{(2)c} e_{(1)b} = 0. \tag{59}$$

Equations (56) and (59) determine $B_{(0)}{}^b$ completely once the initial conditions are assigned on a hypersurface Σ, which is transverse to the rays. In this way we can solve the initial value problem for the set of Eqs. (8)–(12). We assume that on the hypersurface Σ' $A_{(q)}$ and $B_{(q)}$ have been given with $q \geqslant 0$, together with the initial value for the phase Θ. Now we determine $B_{(0)}$, Θ in a neighborhood, $\mathscr{D}$, of Σ where the rays do not intersect (absence of caustics) by integration of (47) and (59).

Finally we solve (53) recursively for $A_{(q)}$ and $B_{(q)}$ in terms of $A_{(q-1)}$ and $B_{(q-1)}$. That this is possible is shown in the appendix, where it is also shown how $N_{(q)}$, $V_{(q)}$, $M_{(q)}$, $\tilde{N}_{(q)}$, $\tilde{V}_{(q)}$, $\tilde{M}_{(q)}$ are known in terms of $A_{(q)}$, $B_{(q)}$. Therefore, we have obtained a solution to the system (8)–(11) in terms of a formal series.

3. FARADAY ROTATION AND CONCLUSIONS

In this section we take into account Faraday rotation. In many astrophysical situations the background plasma is also endowed with a magnetic field. Equation (10) is then replaced by

$$\nabla_a \hat{T}^{ab} + e\hat{n}F^{ab}u_a + en\hat{F}^{ab}u_a + enF^{ab}\hat{u}_a = 0, \tag{10'}$$

where

$$F_{ab} = \eta_{abcd}B^c u^d = Bf_{ab} \tag{60a}$$

with

$$B^a = Bm^a, \quad m_a m^a = 1. \tag{60b}$$

Now we assume that the magnetic field is so weak that it does not affect the dispersion relation (43). That is

$$enF^{ab} = O(\epsilon)$$

we take this into account explicitly by rewriting Eq. (10') as follows:

$$\nabla_a \hat{T}^{ab} + en\hat{F}^{ab}u_a + \epsilon(enBf^{ab})\hat{u}_a = 0. \tag{61}$$

In this way we obtain a modified set of Eqs. (8), (9), (61), (11), (12) which we subject to the same analysis as before. Of course we reobtain the same dispersion relation (43). The propagation equation, however, reads

$$2DB_{(0)}{}^b + l^a{}_{;a}B_{(0)}{}^b - \frac{\omega_p^2}{\Omega f}B_{(0)a}\omega^{ab} + \frac{eB\omega_p^2}{m\Omega f^2}f^{ab}B_{(0)a} + \text{terms lying in the 2-plane spanned by } u^a \text{ and } l^a. \tag{62}$$

Again, contracting (62) with $B_{(0)}{}^b$ we obtain the usual conservation law (56).

Now we introduce the tetrad $\{u^a, \nu^a, e_{(1)}{}^a, e_{(2)}{}^a\}$ as in Sec. 2. Let α be the angle between the vorticity vector $\omega^a = \frac{1}{2}\eta^{abcd}u_b\omega_{cd}$ and the unit vector ν^a. Similarly, let φ be the angle between the magnetic field B^a and ν^a. Proceeding as in Sec. 2, Eq. (62) yields:

$$D\Psi - \frac{\omega_p^2}{2\Omega f}\omega\cos\alpha = \omega_B \frac{\omega_p^2}{2\Omega f}\cos\varphi, \tag{63}$$

where $\omega_B = eB/m$ is the Larmor frequency, and $\omega = (\omega^a\omega_a)^{1/2}$ is the vorticity scalar.

From (63) we see that the effect of vorticity on the polarization angle is analogous to that of Faraday rotation. More precisely, the effect of the vorticity vector is equivalent to that of a magnetic field forming the same angle α with the propagation direction and of strength $B = (m/e)f\omega$.

In a realistic situation both the "vorticity effect" and Faraday rotation would be present. The ratio of these two terms is

$$\frac{\omega f}{\omega_B}$$

and for the vorticity effect to be important a high angular velocity and an ultrarelativistic fluid ($\omega \gg 1, f \gg 1$) are required. This situation might occur near a rapidly rotating black hole. The equivalence between the vorticity and magnetic field is easily understood in simple physical terms in the case $f = 1$. In fact, in an electron gas imbedded in a magnetic field, the electrons revolve around the field lines with an angular velocity ω_B. Therefore, a right-handed circularly polarized wave sees a different refractive index than a left-handed one. This is the physical cause of Faraday rotation. Of course the same effect would be achieved if the electrons were constrained to revolve around the same lines with the same angular velocity $\omega = \omega_B$, in the absence of a background magnetic field.

Now we give a simple example. We consider a homogeneous electron fluid in special relativity. We assume that the medium is endowed with a uniform rigid rotation ω around the z axis and that the wave propagates in the xz plane. In the absence of a background magnetic field Eq. (63) reads

$$\frac{d\psi}{d\sigma} = \left(\frac{\omega}{2\Omega f}\right)\cos\alpha,$$

where σ is defined by

$$\frac{dx^a}{d\sigma} = \frac{1}{\omega_p^2}l^a.$$

Therefore, for propagation perpendicular to the angular velocity vector there is no effect. For a wave traveling in the z direction the effect is maximum. In this case

$$\frac{dz}{d\sigma} = \frac{\Omega}{\omega_p^2} N,$$

where $N=(1-\omega_p^2/\Omega^2)^{1/2}$ is the refractive index of the medium. After the wave has traveled a distance L, its polarization plane is rotated by an angle $\Delta\psi$ which is, in physical units,

$$\Delta\psi=\left(\frac{\omega L}{c}\right)\frac{1}{2fN}\left(\frac{\omega_p^2}{\Omega^2}\right).$$

We see that the effect is likely to be important for sources attaining relativistic speed, $V\sim\omega L\sim c$. Finally we compare our results with those derived by Pichon in a completely different context.[9] Pichon treats the propagation of weak discontinuties in a purely refractive medium, thereby excluding any dispersion. Let us define a phenomenological refractive index $N=(1+l^2/\Omega^2)^{1/2}$. Then Pichon's propagation equations n.(101) reads

$$2K^a\nabla_a e_b - e^a(\nabla_a K_b - \nabla_b K_a)=0, \tag{64}$$

where

$$K_a = l_a + (N^2-1)\Omega\, u_a.$$

If, proceeding as in Sec. 2, we write

$$l_a=\cos\Psi e_{(1)a}+\sin\Psi e_{(2)a},$$

where $e_{(1)a}$ and $e_{(2)a}$ are both orthogonal to each other and u^a, l^a, and furthermore $e_{(2)}{}^b K^a \nabla_a e_{(1)b}=0$, then (64) yields

$$2K^a\nabla_a\Psi + \frac{l^2}{\Omega}\omega^{cb}e_{(2)c}e_{(1)b}=0. \tag{65}$$

which is formally analogous to our Eq. (59). The only difference is that in Eq. (65) the vector K^a appears in place of l^a. This occurs because dispersive effects are neglected in Pichon's analysis. In fact, when dispersive effects are taken into account, albeit in a phenomenological way,[6] the relation between the rays' tangent vector K^a and the phase gradient l^a is given by

$$K^a = l^a + (N^2-1)\Omega\, u^a + N\frac{\partial N}{\partial\Omega}\Omega^2 u^a \tag{66}$$

which, in the particular case $N^2=1-\omega_p^2/\Omega^2$ gives

$$K^a = l^a$$

Finally we conclude with a remark on some cosmological applications. The theory developed in this paper could possibly be applied to the microwave background radiation propagating in the cosmological plasma in a rotating Bianchi universe, thereby obtaining an estimate of the resulting polarization in the microwave background. From the observational upper limits on the amount of polarization one could then infer upper limits on the present vorticity of the universe.

APPENDIX

Theorem: The system of Eqs. (53) together with the initial conditions $A_{(-1)}{}^a = B_{(-1)}{}^a = A_{(0)}{}^a = 0$ can be solved recursively.

Proof: For the sake of simplicity we limit ourselves to the case when the matter can be described by dust, i.e., $T_{ab}=\mu u_a u_b$. The extension to more general forms of matter is straightforward. First of all we express $\tilde{V}_{(p+1)}{}^a$, $\tilde{N}_{(p+1)}$, $V_{(p+1)}{}^a$, $N_{(p+1)}$ in terms of $A_{(q)}{}^a$, $B_{(q)}{}^a$, $q\leqslant p+1$. From Eqs. (50) after some manipulations we obtain:

$$V_{(p+1)}{}^b = \frac{1}{\mu\Omega}\{u_c\tilde{S}_{(p)}{}^{ac}{}_{;a}u^b + \tilde{S}_{(p)}{}^{ab}{}_{;a} + en\,\tilde{\Psi}_{(p+1)}{}^{ab}u_a\}, \tag{A1}$$

$$\tilde{V}_{(p+1)}{}^b = -\frac{1}{\mu\Omega}\{u_c S_{(p)}{}^{ac}{}_{;a}u^b + S_{(p)}{}^{ab}{}_{;a} + en\,\Psi_{(p+1)}{}^{ab}u_a\}, \tag{A2}$$

and from Eqs. (51):

$$N_{(p+1)} = \frac{1}{\Omega}\{-n\,l_a V_{(p+1)}{}^a + [n\,\tilde{V}_{(p)}{}^a + \tilde{N}_{(p)}u^a]_{;a}\}, \tag{A3}$$

$$\tilde{N}_{(p+1)} = -\frac{1}{\Omega}\{n\,l_a\tilde{V}_{(p+1)}{}^a + [n\,V_{(p)}{}^a + N_{(p)}u^a]_{;a}\}. \tag{A4}$$

Further manipulation of (A1)–(A4) together with repeated use of (50) and (51) yields:

$$n\,V_{(p+1)}{}^b = \frac{1}{\Omega}\left\{n\,\tilde{V}_{(p)}{}^a u^b{}_{;a} + n\,u^a\tilde{V}_{(p)}{}^b{}_{;a} + \frac{en}{m}\times[u_a B_{(p)}{}^{b;a} - u_a B_{(p)}{}^{a;b} + \Omega A_{(p+1)}{}^b - l^b(A_{(p+1)}{}^a u_a)]\right\}, \tag{A5}$$

$$N_{(p+1)} = \frac{1}{\Omega}[n\,\tilde{V}_{(p)}{}^a + N_{(p)}u^a]_{;a} - \frac{1}{\Omega^2}\times\left\{n\,\tilde{V}_{(p)}{}^a u^c{}_{;a}l_c + n\,u^a\tilde{V}_{(p)}{}^c{}_{;a}l_c + \frac{en}{m}\times[u_a B_{(p)}{}^{c;a}l_c - u_a D B_{(p)}{}^a \times -l^2(A_{(p+1)}{}^a u_a)]\right\}, \tag{A6}$$

$$n\tilde{V}_{(p+1)}{}^{b}=-\frac{1}{\Omega}\Big\{n V_{(p)}{}^{a}u^{b}{}_{;a}+n u^{a}V_{(p)}{}^{b}{}_{;a}+\frac{en}{m}$$
$$\times[u_{a}A_{(p)}{}^{a;b}-u_{a}A_{(p)}{}^{b;a}+\Omega B_{(p+1)}{}^{b}$$
$$-l^{b}(B_{(p+1)}{}^{a}u_{a})]\Big\}, \tag{A7}$$

$$\tilde{N}_{(p+1)}=-\frac{1}{\Omega}[n V_{(p)}{}^{a}+N_{(p)}u^{a}]_{;a}+\frac{1}{\Omega^{2}}$$
$$\times\Big\{l_{c}V_{(p)}{}^{a}u^{c}{}_{;a}+n u^{a}V_{(p)}{}^{c}{}_{;a}+\frac{en}{m}$$
$$\times[u_{a}DA_{(p)}{}^{a}-u_{a}A_{(p)}{}^{c;a}l_{c}-l^{2}(B_{(p+1)}{}^{a}u_{a})]\Big\}. \tag{A8}$$

Let us indicate by $\tilde{O}(p)$ a quantity containing terms of the kind $A_{(q)}, B_{(q)}$, with $q\leqslant p$ only. Then, by inspection of (A5)–(A8) one finds:

$$n V_{(p)}{}^{b}=\frac{en}{m}\left[A_{(p)}{}^{b}-\frac{1}{\Omega}l^{b}(A_{(p)}{}^{a}u_{a})\right]+\tilde{O}(p-1), \tag{A9}$$

$$N_{(p)}=\frac{en}{m\Omega^{2}}l^{2}(A_{(p)}{}^{a}u_{a})+\tilde{O}(p-1), \tag{A10}$$

$$n\tilde{V}_{(p)}{}^{b}=\frac{en}{m}\left[-B_{(p)}{}^{b}+\frac{1}{\Omega}l^{b}(B_{(p)}{}^{a}u_{a})\right]+\tilde{O}(p-1), \tag{A11}$$

$$\tilde{N}_{(p)}=-\frac{en}{m}\frac{l^{2}}{\Omega^{2}}(B_{(p)}{}^{a}u_{a})+\tilde{O}(p-1). \tag{A12}$$

Substituting into Eq. (53b) yields

$$2DB_{(p)}{}^{b}+l^{a}{}_{;a}B_{(p)}{}^{b}-l^{b}B_{(p)}{}^{a}{}_{;a}$$
$$+\frac{4\pi e}{\Omega}[n\tilde{V}_{(p)}{}^{a}u^{b}{}_{;a}+n u^{a}\tilde{V}_{(p)}{}^{b}{}_{;a}]$$
$$+\frac{4\pi e^{2}n}{m\Omega}(u_{a}B_{(p)}{}^{b;a}-u_{a}B_{(p)}{}^{a;b})$$
$$+\frac{l^{2}}{\Omega}l^{b}(A_{(p+1)}{}^{a}u_{a})+\frac{4\pi e}{\Omega}\Xi_{(p)}+\tilde{O}(p-1)=0, \tag{A13}$$

with

$$\Xi_{(p)}=[n\tilde{V}_{(p)}{}^{a}+\tilde{N}_{(p)}u^{a}]_{;a}$$
$$-\frac{1}{\Omega}[n\tilde{V}_{(p)}{}^{a}u^{c}{}_{;a}l_{c}+n u^{a}\tilde{V}_{(p)}{}^{c}{}_{;a}l_{c}]$$
$$-\frac{en}{m\Omega}[u_{a}B_{(p)}{}^{c;a}l_{c}-u_{a}DB_{(p)}{}^{a}]$$
$$+\frac{en}{\Omega}l^{2}A_{(p+1)}{}^{a}u_{a}. \tag{A14}$$

Let us define

$$W_{(p)}\equiv A_{(p)}{}^{b}u_{b},\quad Z_{(p)}\equiv B_{(p)}{}^{b}u_{b}. \tag{A15}$$

Now we contract Eq. (A13) with u^{b} and get, after some algebra,

$$2DZ_{(p)}-2B_{(p)}{}^{b}Du_{b}+l^{a}{}_{;a}Z_{(p)}-\Omega B_{(p)}{}^{a}{}_{;a}$$
$$+l^{2}W_{(p+1)}-\frac{4\pi e}{\Omega}\Xi_{(p)}+\tilde{O}(p-1)=0. \tag{A16}$$

Contracting (A13) with l^{b} yields

$$-2B_{(0)}{}^{b}Dl_{b}-l^{2}B_{(p)}{}^{a}{}_{;a}+\frac{4\pi e}{\Omega}$$
$$\times\Big[-\frac{en}{m}B_{(p)}{}^{a}u^{b}{}_{;a}l_{b}+\frac{en}{m}l_{b}Du^{b}+\frac{e}{m}$$
$$\times\Big(\frac{1}{\Omega}l^{2}Z_{(p)}\Big)_{;a}u^{a}+\frac{e}{m}B_{(p)}{}^{b}l_{b;a}u^{a}-\frac{e}{m\Omega}u^{a}Dl_{a}\Big]$$
$$+\frac{4\pi e^{2}n}{m\Omega}[-u^{a}B_{(p)}{}^{b}l_{b;a}-DZ_{(p)}+B_{(p)}{}^{a}Du_{a}]$$
$$+\frac{l^{4}}{\Omega}W_{(p+1)}+4\pi e\Xi_{(p)}+\tilde{O}(p-1)=0. \tag{A17}$$

Equations (A16) and (A17) can be solved for $W_{(p+1)}$ and $\Xi_{(p)}$. After substituting into Eq. (A13) one gets, having used (A9),

$$2DB_{(0)}{}^{b}+l^{a}{}_{;a}B_{(p)}{}^{b}+G+\tilde{O}(p-1)=0, \tag{A18}$$

where G is a quantity linear in $B_{(p)}{}^{a}$ and containing terms like $Z_{(p),a}$.

Therefore, in order to solve (A18) we must determine $Z_{(p)}$. In order to do this we consider Eq. (53a) for the value $p-1$ of the suffix. By contracting with u^{b} we get $Z_{(p)}$ in terms of quantities which are $\tilde{O}(p-1)$. Substituting back into (A18) we can then solve for $B_{(p)}{}^{b}$ along the rays, in terms of the initial values of Σ and of quantities of the kind $\tilde{O}(p-1)$. An analogous argument can be applied to Eq. (53a) and leads to similar results.

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Exact occupation statistics of two- and three-dimensional lattices of mixed single particles[a)]

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General expressions are derived which exactly describe the ensemble average number of two or three-dimensional structures per arrangement, created when mixed single particles are arranged on a pure or a mixed lattice. The expressions obtained are applied to the calculation of the number of various mixed nearest-neighbor pairs which are important for various phenomena in multicomponent systems.

I. INTRODUCTION

It was shown in a previous paper[1] that N_z, the exact total number of partial structures created when q indistinguishable single particles are arranged in all possible ways on a lattice of N equivalent sites is given by

$$N_z=\sigma_z\binom{N-z}{q-\alpha}$$

$$=\sigma_z\frac{(N-z)!}{(N-q-z+\alpha)!(q-\alpha)!}, \tag{1}$$

where α denotes the number of particles included in the partial structure consisting of z sites and σ_z is the number of distinguishable ways of placing such a structure on the lattice. Thus the exact ensemble average number of the structure per arrangement, n_z is obtained as

$$n_z=\sigma_z\binom{N-z}{q-\alpha}\binom{N}{q}. \tag{2}$$

These quantities are required for a statistical treatment of various phenomena and have recently been applied to a problem of the heat of adsorption of gas molecule on two-dimensional lattices.[2]

The purpose of the present paper is to derive further general expressions which describe the exact ensemble average number of the structures created when mixed particles of distinguishable single particles are arranged in all possible ways on a pure lattice consisting of indistinguishable sites or a mixed lattice consisting of distinguishable sites, i.e, of different kinds of several sublattices. The expressions obtained are then applied to the calculation of the number of mixed nearest-neighbor pairs which appear on two- or three-dimensional lattices. This knowledge is also required for a statistical treatment of various phenomena of multicomponent systems such as alloys, adsorption of mixed gas molecules, and catalytic chemical reactions on multicomponent solid surfaces.

II. GENERAL EXPRESSION FOR MIXED PARTICLES ON PURE LATTICE

As described previously,[1] when q indistinguishable particles are arranged in all possible ways on a lattice of N equivalent sites, a given structure consisting of α particles plus $z-\alpha$ vacant sites and occupying a particular position on the lattice occurs $\binom{N-z}{q-\alpha}$ times because the $(q-\alpha)$ remaining particles can be arranged in all possible ways on the remaining $N-z$ sites. Now, we consider a system composed of two kinds of single particles whose numbers are given by q_1 and q_2. When q_1 particles are arranged in all possible ways on N sites, a given structure consisting of α_1 particles plus $z-\alpha_1$ vacant sites and occupying a particular position on the lattice occurs $\binom{N-z}{q_1-\alpha_1}$ times. When $q_2-\alpha_2$ particles are arranged on the remaining $N-z-(q_1-\alpha_1)$ sites, further

$$\binom{N-z-(q_1-\alpha_1)}{q_2-\alpha_2}$$

distinguishable ways occur for each of the $\binom{N-z}{q_1-\alpha_1}$ arrangements. Hence, the total number of the structures consisting of $\alpha_1+\alpha_2$ particles plus $z-(\alpha_1+\alpha_2)$ vacant sites and occupying a particular position on the lattice created when q_1+q_2 particles are arranged in all possible ways on N sites is given by

$$\binom{N-z}{q_1-\alpha_1}\binom{N-z-(q_1-\alpha_1)}{q_2-\alpha_2}. \tag{3}$$

From the similar arguments, when q mixed particles of ν kinds are arranged in all possible ways in a lattice, the total number of given structures of z sites composed of α particles plus $z-\alpha$ vacant sites which appear at a particular position in the lattice becomes

$$\binom{N-z}{q_1-\alpha_1}\binom{N-z-(q_1-\alpha_1)}{q_2-\alpha_2}\cdots$$
$$\times\binom{N-z-(q_1-\alpha_1)-\cdots-(q_{\nu-1}-\alpha_{\nu-1})}{q_\nu-\alpha_\nu}$$
$$=\prod_{j=1}^{\nu}\binom{N-z-\sum_{k=1}^{j-1}(q_k-\alpha_k)}{q_j-\alpha_j}, \tag{4}$$

where $q=\Sigma_\nu^{j=1}q_j$ and $\alpha=\Sigma_\nu^{j=1}\alpha_j$, There are σ_z distinguishable ways of placing such a structure on the lattice and the quantity (4) is independent of the position for the present case of single particles, i.e., $\lambda=1$, where λ refers to the number of contiguous lattice sites occupied by a particle. Therefore, N_z, the total number of such structures created when q

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mixed particles of ν kinds are arranged in all possible ways on N equivalent sites is

$$N_z=\sigma_z\prod_{j=1}^{\nu}\binom{N-z-\sum_{k=1}^{j-1}(q_k-\alpha_k)}{q_j-\alpha_j}. \tag{5}$$

On the other hand, W, the total number of distinguishable ways in which q mixed particles of ν kinds are arranged in all possible ways on a lattice of N equivalent sites is given by

$$W=\frac{N!}{(N-q)!\prod_{j=1}^{\nu}q_j!}$$

$$=\prod_{j=1}^{\nu}\binom{N-\sum_{k=1}^{j-1}q_k}{q_j}. \tag{6}$$

Thus the exact ensemble average number of the structures per arrangement, n_z, is

$$n_z=\frac{N_z}{W}$$

$$=\sigma_z\prod_{j=1}^{\nu}\binom{N-z-\sum_{k=1}^{j-1}(q_k-\alpha_k)}{q_j-\alpha_j}\Big/\prod_{j=1}^{\nu}\binom{N-\sum_{k=1}^{j-1}q_k}{q_j}, \tag{7}$$

which leads to

$$n_z=\sigma_z[q_1(q_1-1)\cdots(q_1-\alpha_1+1)\,][q_2(q_2-q_1)\cdots$$

$$\times(q_2-\alpha_2+1)\,]\cdots[q_\nu(q_\nu-1)\cdots(q_\nu-\alpha_\nu+1)\,]$$

$$\times(N-q_1-q_2-\cdots-q_\nu)(N-q_1-q_2-\cdots-q_\nu-1)$$

$$\cdots(N-q_1-q_2-\cdots-q_\nu-z+\alpha_1+\cdots+\alpha_\nu+1)$$

$$\times[N(N-1)(N-2)\cdots(N-z+1)\,]^{-1} \tag{8}$$

for $N\neq\sum_{j=1}^{\nu}q_j$, and

$$n_z=\sigma_z[q_1(q_1-1)\cdots(q_1-\alpha_1+1)\,][q_2(q_2-1)\cdots$$

$$\times(q_2-\alpha_2+1)\,]\cdots[q_\nu(q_\nu-1)\cdots(q_\nu-\alpha_\nu+1)\,]$$

$$\times[N(N-1)(N-2)\cdots(N-z+1)\,]^{-1} \tag{9}$$

for $N=\sum_{j=1}^{\nu}q_j$.

III. MIXED NEAREST-NEIGHBOR PAIRS ON PURE LATTICES

In this section we consider the ensemble average number of several mixed nearest-neighbor pairs per arrangement, created when mixed single particles are arranged in all possible ways on a two-dimensional $(R\times S)$-rectangular lattice and a three-dimensional $(R\times S\times T)$-rectangular parallelelpiped lattice whose three axes are composed of R, S, and T sites.

A. Mixed nearest-neighbor pairs on $(R\times S)$-rectangular lattice

σ_z for a similar $(r\times s)$-rectangular structure forming on the lattice is given by[1]

$$\sigma_z=(R-r+1)(S-s+1)+(R-s+1)(S-r+1) \tag{10}$$

for $r\neq s$. Hence, for instance, the exact ensemble average number per arrangement of mixed first-nearest-neighbor pairs of different kinds of particles 1 and 2 (n_{12}), numbers of the mixed third-nearest-neighbor pairs with (n_{112}) and without (n_{102}) intervening particle created when q mixed particles of ν kinds are arranged in all possible ways may be derived respectively by setting $[r=2, s=1, \alpha_1=\alpha_2=1, \alpha_j=0(j=3, 4,\cdots\nu)]$,$[r=3, s=1, \alpha_1=2, \alpha_2=1, \alpha_j=0(j=3, 4,\cdots,\nu)]$ and $[r=3, s=1, \alpha_1=\alpha_2=1,\alpha_j=0(j=3, 4,\cdots,\nu)]$ in Eq. (8) and (10) with $N=RS$ and $z=rs$, as

$$n_{12}=2(2RS-R-S)\,\frac{q_1q_2}{RS(RS-1)}, \tag{11}$$

$$n_{112}=2(2RS-2R-2S)\,\frac{q_1(q_1-1)q_2}{RS(RS-1)(RS-2)}, \tag{12}$$

and

$$n_{102}=2(2RS-2R-2S)\,\frac{q_1q_2(RS-q)}{RS(RS-1)(RS-2)}, \tag{13}$$

where the factor 2 prior to the brackets in (11)–(13) arises from interchangeability between the particles 1 and 2 in the mixed nearest-neighbor pairs.

Further, the σ_z for a linear array of r contiguous sites along diagonals is given by[1]

$$\sigma_z=2(R-r+1)(S-r+1). \tag{14}$$

Thus, n'_{12}, the exact ensemble average number of the second-nearest-neighbor pairs (i.e., the first-nearest-neighbor pairs along a diagonal) per arrangement is obtained by setting $[z=r=2, \alpha_1=\alpha_2=1, \alpha_j=0(j=3,4,\cdots,\nu)\,]$ in (8) and (14) as

$$n'_{12}=4(R-1)(S-1)\,\frac{q_1q_2}{RS(RS-1)}. \tag{15}$$

The ensemble average numbers of these nearest-neighbor pairs per site (n_z/N) corresponding to the (11)–(13) and (15) lead to $4\theta_1\theta_2$, $4\theta_1^2$, $4\theta_1\theta_2(1-\theta)$, and $4\theta_1\theta_2$, respectively, in the limit as R and S approach infinity, where θ denotes surface coverage defined by $\theta=q/RS$ and $\theta_j=q_j/RS$. These limiting quantities have been used in the term of "Langmuir–Hinshelwood mechanism" for kinetical analysis of catalytic reactions involved in several kinds of adsorbed species on a solid surface. Now I have derived the exact relations which are particularly useful for the analysis of surface reactions on crystalline lattices so small that the sites of corners or edges in the lattices cannot be neglected.

B. Mixed nearest-neighbor pairs in a $(R\times S\times T)$-three-dimensional parallelepiped lattice

First we consider the σ_z for a $(r\times s\times t)$-parallelepiped type structure forming in a similar type of $(R\times S\times T)$-parallelepiped lattice. In this case, there are $(R-r+1)(S-s+1)(T-t+1)$ distinguishable ways of placing the structure in the lattice, of which $(R-r+1)$ are of one kind along an axis among the three axes, and $(S-s+1)$ or $(T-t+1)$ the other along the second or third axis. Thus,

$$\sigma_z=(R-r+1)(S-s+1)(T-t+1)+(R-s+1)$$
$$\times(S-r+1)(T-t+1\ )+(R-r+1)(S-t+1)$$
$$\times(T-s+1)+(R-t+1)(S-s+1)(T-r+1) \quad (16)$$

for $r\neq s\neq t$,

$$\sigma_z=(R-r+1)(S-r+1)(T-t+1)+(R-t+1)(S-r+1)$$
$$\times(T-r+1)+(R-r+1)(S-t+1)(T-r+1) \quad (17)$$

for $r=s\neq t$, and

$$\sigma_z=(R-r+1)(S-r+1)(T-r+1) \quad (18)$$

for $r=s=t$. Hence, the exact ensemble average number of the mixed first-nearest-neighbor pairs of particles per arrangement, $n_{III\text{-}12}$, created when q particles of ν kinds are arranged in all possible ways in a $(R\times S\times T)$-superlattice (i.e., $N=\Sigma_\nu^{j=1}q_j$) is obtained by setting $[r=s=1,\ t=2,\ \alpha_1=\alpha_2=1,\ \alpha_j=0\ (j=3,4,\cdots,\nu)]$ in Eqs. (9) and (17) with $N=RST$ and $z=rst$ as

$$n_{III\text{-}12}=2(3RST-RS-RT-ST\ )\frac{q_1q_2}{RST(RST-1)}. \quad (19)$$

Further, the σ_z for a linear array of r-contiguous sites along diagonals through the second- or third-nearest-neighbor sites in the lattice is obtained respectively as

$$\sigma_z=2\ [(R-r+1)(S-r+1)T$$
$$+(R-r+1)(T-r+1)S$$
$$+(S-r+1)(T-r+1)R\ ] \quad (20)$$

or

$$\sigma_z=4(R-r+1)(S-r+1)(T-r+1), \quad (21)$$

where the factor 2 or 4 arises because there are two or four distinguishable directions of the diagonals respectively in the lattice. Thus, the ensemble average number of the mixed second-and third-nearest-neighbor pairs (i.e, first- and second nearest-neighbor pairs along diagonals) are derived by setting $[r=2,\ \alpha_1=\alpha_2=1,\ \alpha_j=0\ (j=3,4,\cdots,\nu)]$ in Eqs. (9), (20), and (21), respectively as

$$n_{III\text{-}12}=4[3RST-2(RS+RT+ST)$$
$$+R+S+T\ ]\frac{q_1q_2}{RST(RST-1)} \quad (22)$$

and

$$n''_{III\text{-}12}=8(R-1)(S-1)(T-+)$$
$$\times\frac{q_1q_2}{RST(RST-1)}, \quad (23)$$

where the interchangeability between the particles 1 and 2 is also taken into account. These quantities (19), (22), and (23) lead to $\phi q_1q_2/N$ when R, S and $T\gg 1$, where ϕ denotes the coordination number of the corresponding nearest-neighbor site.

IV. GENERAL EXPRESSION FOR MIXED PARTICLES ON MIXED LATTICE

In this section we derive a general expression which describes exactly the ensemble average number of the structures created when q mixed particles of ν kinds are arranged in all possible ways on a lattice composed of κ different kinds. This is closely associated with order-disorder problems in alloys.

When N_i is the number of sites of the sublattice of ith kind and $q_{i,j}$ the number of particles of jth kind which occupy the sublattice of ith kind, W (the total number of distinguishable ways in which q such mixed particles of ν kinds are arranged in all possible ways on the lattice consisting of κ sublattices) is given by

$$W=\prod_{i=1}^{\kappa}\frac{N_i!}{(N_i-\sum_{j=1}^{\nu}q_{i,j})!\prod_{j=1}^{\nu}q_{i,j}!}$$
$$=\prod_{i=1}^{\kappa}\prod_{j=1}^{\nu}\binom{N_i-\sum_{k=1}^{j-1}q_{i,k}}{q_{i,k}}. \quad (24)$$

From the similar arguments to those described in Sec. II, the total number of given structures composed of z sites appeared in such W arrangements is obtained as

$$N_z=\sigma_z\binom{N_1-z_1}{q_{1,1}-\alpha_{1,1}}\binom{N_1-z_1-(q_{1,1}-\alpha_{1,1})}{q_{1,2}-\alpha_{1,2}}$$
$$\cdots\binom{N_1-z_1-\sum_{k=1}^{\nu-1}(q_{1,k}-\alpha_{1,k})}{q_{1,\nu}-\alpha_{1,\nu}}\binom{N_2-z_2}{q_{2,1}-\alpha_{2,1}}$$

$$\times \binom{N_2 - z_2 - (q_{2,1} - \alpha_{2,1})}{q_{2,2} - \alpha_{2,2}} \cdots \binom{N_2 - z_2 - \sum_{k=1}^{\nu-1} (q_{2,k} - \alpha_{2,k})}{q_{2,\nu} - \alpha_{2,\nu}}$$

$$\times \binom{N_\kappa - z_\kappa}{q_{\kappa,1} - \alpha_{\kappa,1}} \binom{N_\kappa - z_\kappa - (q_{\kappa,1} - \alpha_{\kappa,1})}{q_{\kappa,2} - \alpha_{\kappa,2}}$$

$$\cdots \binom{N_\kappa - z_\kappa - \sum_{k=1}^{\nu-1} (q_{\kappa,k} - \alpha_{\kappa,k})}{q_{\kappa,\nu} - \alpha_{\kappa,\nu}}$$

$$= \sigma_z \prod_{i=1}^{\kappa} \prod_{j=1}^{\nu} \binom{N_i - z_i \sum_{k=1}^{j-1} (q_{i,k} - \alpha_{i,k})}{q_{i,j} - \alpha_{i,j}}, \tag{25}$$

where z_i denotes the number of sites in the structure which occupy the sublattice of ith kind and $\alpha_{i,j}$ is the number of particles of jth kind contained in the z_i sites, therefore

$$z = \sum_{i=1}^{\kappa} z_i \text{ and } \alpha = \sum_{i=1}^{\kappa} \sum_{j=1}^{\nu} \alpha_{ij}.$$

Thus, the ensemble average number of the structures of z sites per arrangement in this case is expressed by

$$\sigma_z \prod_{i=1}^{\kappa} \prod_{j=1}^{\nu} [q_{ij}(q_{ij} - 1) \cdots \times (q_{ij} - \alpha_{ij} + 1)\,][(N_i - q_i)(N_i - q_i - 1) \cdots \times (N_i - q_i - z_i + \alpha_i + 1)\,][N_i(N_i - 1) \cdots \times (N_i - z_i + 1)\,]^{-1}, \tag{26}$$

where $q_i = \sum_{j=1}^{\nu} q_{ij}$ and $\alpha_i = \sum_{j=1}^{\nu} \alpha_{ij}$, and when $N_i = q_i$ $(i = 1, 2, \cdots, \kappa)$, (26) leads to

$$\sigma_z \prod_{i=1}^{\kappa} \prod_{i=1}^{\nu} [q_{ij}(q_{ij} - 1) \cdots \times (q_{ij} - \alpha_{ij} + 1)\,][N_i(N_i - 1) \cdots \times (N_i - z_i + 1)\,]^{-1}. \tag{27}$$

Now we apply the expression (27) to a binary alloy of a NaCl type rectangular $(R \times S \times T)$-parallelepiped. In this case the ensemble average number of the mixed first-nearest-neighbor pairs of particles per arrangement is obtained by setting $[\kappa = \nu = 2, N_1 = N_2 = \nu/2$, and $(\alpha_{1,1} = \alpha_{2,2} = 1, \alpha_{1,2} = \alpha_{2,1} = 0)$ or $(\alpha_{1,2} = \alpha_{2,1} = 1, \alpha_{1,1} = \alpha_{2,2} = 0)]$ in (27) with $\sigma_z = 3RST - RT - ST - RS$ as

$$(3RST - RS - RT - ST)\left(\frac{q_{1,1}q_{2,2}}{N_1 N_2} + \frac{q_{1,2}q_{2,1}}{N_1 N_2}\right). \tag{28}$$

If we introduce the term "degree of long range order" s', then we have

$$\frac{(1+s')}{2} = \frac{q_{1,1}}{N_1} = \frac{q_{2,2}}{N_2} \quad \text{and}$$
$$\frac{(1-s')}{2} = \frac{q_{1,2}}{N_1} = \frac{q_{2,1}}{N_2}. \tag{29}$$

Using these relations, (28) leads to

$$(3RST - RS - RT - ST)(1 + s'^2)/2, \tag{30}$$

which is the exact expression of the ensemble average number of the mixed first-nearest-neighbor pairs of particles derived within the framework of random distribution. The quantity (30) gives $3N(1 + s'^2)/2$ in the limit as R, S, and T approach infinity, which is equivalent to the value derived previously by approximate method.[3]

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Multipole wavefunctions for photoelectrons in crystals. IV. The irregular functions and the matching to an impurity[a)]

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Extension of the method of partial waves to scattering by an impurity center in a crystal requires the construction of energy eigenfunctions of the unperturbed crystal that are irregular at the center. These irregular solutions of a nonseparable problem are constructed by utilizing the expansion of the Green's function into the regular solutions symmetry-adapted about the impurity center, which have been obtained earlier. The wavefunction within an impurity can thus be continued throughout the surrounding crystal by matching it at the impurity boundary to a superposition of regular and irregular solutions. This procedure is compared to the current EXAFS treatment of photoabsorption.

I. INTRODUCTION

This paper develops a mathematical framework for matching the wavefunctions of a localized impurity and of its surrounding unperturbed crystalline medium. The matching constitutes the interface for connecting atomic and band properties. Our method extends to crystals the partial wave expansion which is familiar for spherical symmetry. This paper deals with certain aspects of the solutions of the Schrödinger equation with potential fields that possess point group symmetry about an impurity center as well as translational crystal symmetry except for the presence of this center.

We divide the crystal into an *internal* region where the perturbing potential is effective, and an *external* region where the crystal is unperturbed. In previous papers[1-4] we considered a complete set of solutions in the external region, symmetry-adapted to the point group, which remain bounded when continued into the center of the internal region. For this reason we call them *regular* multipole wavefunctions. However, the matching of an impurity wavefunction and of its normal derivative at the boundary of the internal region requires also the knowledge of the corresponding set of *irregular* multipole wavefunctions, that is, of functions which would become singular when continued into the center of the internal region. The construction of these irregular functions constitutes the main task of this paper.

The regular multipole wavefunctions result from a unitary transformation of the Bloch waves with real $\mathbf{k}$ vectors,[3] analogous to the construction of the spherical Bessel functions by superposition of plane waves. Irregular multipole wavefunctions could then be constructed by analogy to the corresponding construction of the spherical Neumann functions, namely, by the integral representation in terms of plane waves,

$$n_l(kr)=\frac{1}{4i^{l+1}}\int_C d\Theta \sin\Theta\ e^{ikr\cos\Theta}P_l(\cos\Theta), \qquad (I.1)$$

where C is a suitable path in the complex Θ plane.[5] However, in the crystal situation the nonseparability of angular variables makes it difficult to identify the appropriate path in the three-dimensional complex domain of $\mathbf{k}$ vectors. Moreover, even though Bloch waves with complex $\mathbf{k}$ vectors can be defined by analytic continuation,[6] degeneracies among bands make their constructive definition unpractical. On the other hand, the Neumann functions can also be defined by a Green's function formalism,[7] which depends only on general properties of partial differential equations rather than on the separation of variables for spherical symmetry. Extension of this procedure proves feasible.

In spherical symmetry a wavefunction can be expanded into spherical partial waves in both the internal and the external region. The matching at the spherical boundary can thus be performed by considering one partial wave at a time, working with radial wavefunctions only. An equivalent statement is that the portion of the boundary contained in the *basic domain*[8] in spherical symmetry reduces to a single point, so that it suffices to perform the matching at any one reference point on the sphere, the symmetry taking care of the rest. When the symmetry is lowered to a point group, the portion of the boundary surface contained in the basic domain has *finite* extension; an *infinite* number of functions is then needed to perform the matching for each symmetry species.

The impurity wavefunction in the internal region could be calculated by an extension of the cellular method of band theory, e.g., in the formulation of Altmann *et al.*[9] Alternatively, a variational calculation within the internal region would apply regardless of nonsphericity of the internal region, and, most of all, would also enable one to treat the internal region as a many-particle problem. This approach to the impurity problem in crystals would thus eventually converge to an R-matrix calculation.[10]

Full specification of the impurity potential would require taking into account the relaxation of the medium about the impurity so as to screen completely the effect of the impurity outside the internal region. This problem exceeds the scope of this paper and will be treated separately.

The plan of the paper is as follows. Section II summarizes properties of the regular multipole wavefunctions. Section III solves the one-electron Schrödinger equation with

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an impurity center formally, while Sec. IV recasts the solutions in a form that holds in the external region only. Section V introduces a set of harmonics of the boundary of the internal region. The matching of the impurity wavefunction and of its normal derivative is treated in Sec. VI. Section VII compares the present approach with current EXAFS theories of photoabsorption.

II. PROPERTIES OF THE REGULAR MULTIPOLE WAVEFUNCTIONS

This section summarizes properties of the regular multipole wavefunctions $\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r};E_\mu)$ to be used in the following and discusses their analytic dependence on the energy E.

The $\mathscr{R}$ functions are obtained by unitary transformation of the set of Bloch waves $\varphi_\mu(\mathbf{r};\mathbf{k})$ with energy $E_\mu(\mathbf{k})=E$[3]:

$$\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r};E_\mu)$$

$$=\frac{1}{i^L\Omega^{1/2}}\int_\Omega d\,\mathbf{k}\delta[E-E_\mu(\mathbf{k})]\varphi_\mu(\mathbf{r};\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{t}_\mu)$$

$$\times\sum_{i'=1}^{\dim(\Gamma')}P_{Lq}^{(\Gamma' i')}(\mathbf{k};E_\mu)(\Gamma' i',\ \Gamma(\mu)|\Gamma i), \tag{II.1}$$

where Ω stands both for the Brillouin zone and for its volume. The coupling coefficients $(\Gamma' i',\ \Gamma(\mu)|\Gamma i)$, which were implied but not explicitly indicated in Ref. 4, serve to reduce the Kronecker product representation $\Gamma(\mu)\times\Gamma'(\mu)$ being the one-dimensional irreducible representation of the Wannier function $a_\mu(\mathbf{r})$.[4] As in Refs. 3 and 4, we confine ourselves to crystals with a single atom per unit cell and with the atom at the cell's center. The role of the various factors in the integral of Eq. (II.1) and the specification of the phase of the Bloch waves have been discussed in Ref. 4. We need only to recall here that the functions $\mathscr{R}$:

(i) are real, that is, they correspond to standing-wave type solutions of the unperturbed crystal Hamiltonian, H_0;

(ii) transform according to the ith row of the irreducible representation Γ of the crystal point group acting at $\mathbf{r}=0$, that is, at the position of the impurity;

(iii) are normalized according to

$$\int d\,\mathbf{r}\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r};E_\mu)\,\mathscr{R}_{Lq'}^{(\Gamma i)}(\mathbf{r};E'_{\mu'})$$

$$=\delta(E-E')\ \delta_{\mu\mu'}\delta_{LL'}\delta_{qq'}, \tag{II.2}$$

where the integration extends over the whole (infinite) crystal;

(iv) are complete in the sense that

$$\sum_\mu\int_{\min(E_\mu)}^{\max(E_\mu)}dE\sum_{\Gamma iLq}\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r};E_\mu)\,\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r}';E_\mu)=\delta(\mathbf{r}-\mathbf{r}'). \tag{II.3}$$

The factor i^{-L} has been included, as noted in Sec. X of Ref. 4, to make the $\mathscr{R}$ real.

The $\mathscr{R}$ functions have an alternative representation in terms of Wannier functions[4]:

$$\mathscr{R}_{Lq}^{(\Gamma i)}(\mathbf{r};E_\mu)$$

$$=\sum_{\mathbf{n}}a_\mu(\mathbf{r}-\mathbf{n})\sum_{i'=1}^{\dim(\Gamma')}\langle\mathbf{n}+\mathbf{t}_\mu|\Gamma' i' Lq\rangle_{E_\mu}$$

$$\times(\Gamma' i',\ \Gamma(\mu)|\Gamma i), \tag{II.4}$$

with coefficients (called *lattice multipoles*)

$$\langle\mathbf{n}+\mathbf{t}_\mu|\Gamma' i' Lq\rangle\equiv\frac{1}{i^L\Omega}$$

$$\times\int_\Omega d\,\mathbf{k}\delta[E-E_\mu(\mathbf{k})]P_{Lq}^{(\Gamma' i')}(\mathbf{k};E_\mu)\exp[i\mathbf{k}\cdot(\mathbf{n}+\mathbf{t}_\mu)]. \tag{II.5}$$

These coefficients converge to zero for any given $\mathbf{n}$

$$\lim_{L\to\infty}|\langle\mathbf{n}+\mathbf{t}_\mu|\Gamma' i' Lq\rangle_{E_\mu}|=0, \tag{II.6}$$

and for any given L

$$|\langle\mathbf{n}+\mathbf{t}_\mu|\Gamma' i' Lq\rangle_{E_\mu}|=O(1/|\mathbf{n}|). \tag{II.7}$$

One may also show that

$$|\langle\mathbf{n}+\mathbf{t}_\mu|\Gamma' i' Lq\rangle_{E_\mu}|\leq[D_\mu(E)]^{1/2}G_L^{(\Gamma')}(|\mathbf{n}+\mathbf{t}_\mu|), \tag{II.8}$$

where $D_\mu(E)$ is the density of states of the unperturbed crystal contributed by the μth band per crystal cell, and $G_L^{(\Gamma')}(|\mathbf{n}+\mathbf{t}_\mu|)$ is a geometrical factor. This factorization permits one to show that lattice multipoles with high L have vanishing amplitude in the proximity of the central cell, $\mathbf{n}=0$. Moreover, because, for small $|\mathbf{r}|$, $\lim_{|\mathbf{n}|\to\infty}|a_\mu(\mathbf{r}-\mathbf{n})|=0$, we expect that the *$\mathscr{R}$ functions with high L will also have vanishing amplitude for small $|\mathbf{r}|$*, say on the boundary of the internal zone. The maximum value of L, $L_{\max}$, that one needs to consider will then depend essentially on the convergence of the Wannier expansion (II.4).

The series (II.4) is uniformly convergent over the interval $[\min(E_\mu),\ \max(E_\mu)]$. The $\mathscr{R}$ functions are, therefore, *continuous* functions of E in that interval and vanish at the band edges. One can also show that the lattice multipoles (II.5) are analytic functions of E within the range of the band except at critical energies E_C where they exhibit singularities not worse than those of the density of states $D_\mu(E)$.[11] We can consider the $\mathscr{R}$ functions to have the same dependence on E as the lattice multipoles because, for practical applications the series (II.4) will include a finite number of terms.

III. THE SCATTERING BY AN IMPURITY

Our task is to solve the one-electron Schrödinger equation

$$(H_0+V)\,\Psi_{\epsilon,\lambda}^{(\Gamma i)}(\mathbf{r})=\epsilon\Psi_{\epsilon,\lambda}^{(\Gamma i)}(\mathbf{r}), \tag{III.1}$$

where H_0 is the Hamiltonian of the unperturbed crystal and V is the perturbing impurity potential. V is assumed to be nonvanishing in the internal region only, as discussed in the Introduction, and to possess the point group symmetry of the crystal about $\mathbf{r}=0$. The discrete index λ distinguishes

eigensolutions with the same energy ϵ and symmetry species Γi. In this Section we will solve Eq. (III.1) in a formal way by adapting standard techniques of scattering theory. In Sec. IV we will specialize the solutions to a form that holds in the external region only.

Because the $\mathscr{R}$ functions form a complete system and because the perturbing potential V possesses the crystal point group symmetry, we can represent each $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ by an expansion into $\mathscr{R}$ functions belonging to the same symmetry species:

$$\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r}) = \sum_{\mu} \int_{\min(E_\mu)}^{\max(E_\mu)} dE \times \sum_{Lq} \mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};E_\mu)\, D^{(\Gamma i)}_{Lq,\lambda}(E_\mu;\epsilon), \tag{III.2}$$

thus reducing the Schrödinger equation (III.1) to the form

$$(E'-\epsilon)\, D^{(\Gamma i)}_{Lq',\lambda}(E'_{\mu'};\epsilon) + \sum_{\mu} \int_{\min(E_\mu)}^{\max(E_\mu)} dE \times \sum_{Lq} \langle Lq', E'_{\mu'}|V|Lq,E_\mu\rangle^{(\Gamma i)} D^{(\Gamma i)}_{Lq,\lambda}(E_\mu;\epsilon) = 0. \tag{III.3}$$

Here we have set

$$\langle Lq', E'_{\mu'}|V|Lq, E_\mu\rangle^{(\Gamma i)} \equiv \int d\mathbf{r}\, \mathscr{R}^{(\Gamma i)}_{Lq'}(\mathbf{r};E'_{\mu'}) V \mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};E_\mu), \tag{III.4}$$

where the range of V limits the integration to the internal region.

We are interested in *values of ϵ within the allowed range of a band*. The quantity $(E'-\epsilon)$ in Eq. (III.3) may, therefore, vanish. Equation (III.3) can thus be cast in the form of a linear integral equation[12]

$$D^{(\Gamma i)}_{Lq',\lambda}(E'_{\mu'};\epsilon) = \delta(\epsilon-E')\, \alpha^{(\Gamma i)}_{Lq',\lambda}(\epsilon_{\mu'}) + \frac{\mathscr{P}}{(\epsilon-E')} \sum_{\mu} \times \int_{\min(E_\mu)}^{\max(E_\mu)} dE \sum_{Lq} \langle Lq', E'_{\mu'}|V|Lq, E_\mu\rangle^{(\Gamma i)} \times D^{(\Gamma i)}_{Lq,\lambda}(E_\mu;\epsilon), \tag{III.5}$$

where $\mathscr{P}$ means that the principal part is to be taken in any integration over the singularity, and the coefficients α are to be determined by boundary conditions. Equation (III.5) generates an infinite Neumann's series,[13] and its formal solution is

$$D^{(\Gamma i)}_{Lq',\lambda}(E'_{\mu'};\epsilon) = \delta(\epsilon-E')\, \alpha^{(\Gamma i)}_{Lq',\lambda}(\epsilon_{\mu'}) + \frac{\mathscr{P}}{(\epsilon-E')} \times \sum_{\{\mu\}_\epsilon} \sum_{Lq} \langle Lq', E'_{\mu'}|K|Lq,\epsilon_\mu\rangle^{(\Gamma i)} \times \alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu). \tag{III.6}$$

Here the symbol $\{\mu\}_\epsilon$ means that the summation is extended only to those bands whose energy range includes ϵ. Equation (III.6) defines the K matrix.[14] The two terms on the right-hand side of Eq. (III.6) represent contributions "on the energy shell" and "off the energy shell," respectively.

We now insert the solution (III.6) into the expansion (III.2) and get

$$\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r}) = \sum_{\{\mu\}_\epsilon} \sum_{Lq} \tilde{\mathscr{R}}^{(\Gamma i)}_{Lq}(\mathbf{r};\epsilon_\mu)\, \alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu), \tag{III.7}$$

where

$$\tilde{\mathscr{R}}^{(\Gamma i)}_{Lq}(\mathbf{r};\epsilon_\mu) = \mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};\epsilon_\mu) + \sum_{\mu'} \mathscr{P} \int_{\min(E_{\mu'})}^{\max(E_{\mu'})} dE' \sum_{Lq'} \mathscr{R}^{(\Gamma i)}_{Lq'}(\mathbf{r};E'_{\mu'}) \times \frac{1}{\epsilon-E'} \langle Lq', E'_{\mu'}|K|Lq,\epsilon_\mu\rangle^{(\Gamma i)}. \tag{III.8}$$

(The principal-value integrals in this equation and in the following are mathematically well defined for all ϵ within a band owing to the analytical behavior of the $\mathscr{R}$ as functions of E. Furthermore, integrals of this type have been evaluated numerically without difficulty.)[15] The effect of the impurity is thus to modify each $\mathscr{R}$ function with energy ϵ by adding to it the second term of Eq. (III.8), which consists of functions $\mathscr{R}(E')$ with $E' \neq \epsilon$, and hence orthogonal and linearly independent of $\mathscr{R}(\epsilon)$ itself.

The orthonormalization condition of the functions $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ can be worked out either by using operator techniques, as in Ref. 14, or, more directly, by using Eq. (III.5). Attention must be then paid when integrating through the double principal part singularity, as shown in detail in Appendix A of Ref. 16. The result is:

$$\int d\mathbf{r}\, \Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r}) \Psi^{(\Gamma i)}_{\epsilon',\lambda'}(\mathbf{r}) = \sum_{\mu} \int_{\min(E_\mu)}^{\max(E_\mu)} dE \sum_{Lq} D^{(\Gamma i)}_{Lq,\lambda}(E_\mu;\epsilon)\, D^{(\Gamma i)}_{Lq,\lambda'}(E_\mu;\epsilon') = \delta(\epsilon-\epsilon') \sum_{\{\mu\}_\epsilon} \sum_{Lq} [\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\, \alpha^{(\Gamma i)}_{Lq,\lambda'}(\epsilon_\mu) + \beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\, \beta^{(\Gamma i)}_{Lq,\lambda'}(\epsilon_\mu)], \tag{III.9}$$

where

$$\beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\equiv\pi\sum_{|\mu'|_\epsilon}\sum_{Lq'}\langle Lq,\epsilon_\mu|K|Lq',\ \epsilon_{\mu'}\rangle^{(\Gamma i)}\alpha^{(\Gamma i)}_{Lq',\lambda}\ (\epsilon_{\mu'}). \tag{III.10}$$

The eigenfunctions $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ are thus properly orthonormalized by setting

$$\alpha_\lambda(\epsilon)\cdot\alpha_{\lambda'}(\epsilon)+\beta_\lambda(\epsilon)\cdot\beta_{\lambda'}(\epsilon)=\delta_{\lambda\lambda'} \tag{III.11}$$

at each ϵ, where $\alpha_\lambda(\epsilon)\equiv\{\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\}$. Note that we have taken the coefficients α of the expansion (III.7) to be real. The β's, which are defined in terms of the real and symmetric K matrix on the energy shell,[14] are then real, too.

IV. SYMMETRY-ADAPTED GREEN'S FUNCTIONS AND IRREGULAR FUNCTIONS

In Sec. III we have represented the eigenfunctions of the full Hamiltonian H_0+V in a form [Eq. (III.7)] that holds *everywhere* in space, that is, both in the internal and the external region. In this Sec. we recast Eq. (III.7) into a more compact form that holds *in the external region only*. The internal region will be treated instead by a different approach.

We start by rewriting the elementary solutions (III.8) into the equivalent form:

$$\tilde{\mathscr{R}}^{(\Gamma i)}_{Lq}(\mathbf{r};\epsilon)=\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)+\int d\mathbf{r}'G^{(\Gamma i)}_\epsilon(\mathbf{r};\mathbf{r}')\,V\tilde{\mathscr{R}}^{(\Gamma i)}_{Lq}(\mathbf{r}';\ \epsilon_\mu). \tag{IV.1}$$

Here $G^{(\Gamma i)}_\epsilon(\mathbf{r};\mathbf{r}')$ is the *symmetry-adapted principal-value* Green's function

$$G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')=\sum_\mu\mathscr{P}\int_{\min(E_\mu)}^{\max(E_\mu)}dE\times\sum_{Lq}\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};E_\mu)\frac{1}{\epsilon-E}\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r}';E_\mu). \tag{IV.2}$$

This function is symmetry-adapted in that it transforms acording to the ith row of the irreducible representation Γ of the crystal point group under group transformations of *either* $\mathbf{r}$ *or* $\mathbf{r}'$. Since the Green's function is singular at $\mathbf{r}=\mathbf{r}'$, the bilinear expression on the right-hand side of Eq. (IV.2) converges to $G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')$ in the distribution sense, that is, only when integrated over some test function.

Equation (IV.2) constitutes an eigenfunction expansion of the Green's function $G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')$. In the usual context of problems fully separable, e.g., in spherical coordinates, the Green's function can be represented *either* by an expansion analogous to Eq. (IV.2) *or*, alternatively, in its "closed form," i.e., as product of the regular and the irregular solutions of a one-dimensional equation.[17] For instance, when H_0 is the free space Hamiltonian,

$$\frac{1}{rr'}g_l(r;\ r')=\frac{2}{\pi}\mathscr{P}\int_0^\infty dk'\,j_l(kr)\ \frac{k'^2}{k^2-k'^2}j_l(kr')=kn_l(kr)j_l(kr'),\quad r>r'. \tag{IV.3}$$

We want to generalize Eq. (IV.3) to the crystal situation where the variables cannot be separated.

The following considerations hold irrespectively of separation of variables:

(i) Owing to the definition, Eq. (IV.2), and to the completeness of the $\mathscr{R}$ functions, Eq. (II.2), the full principal-value Green's function

$$G_\epsilon(\mathbf{r};\ \mathbf{r}')=\sum_{\Gamma i}G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}') \tag{IV.4}$$

satisfies the inhomogeneous equation

$$(H_0-\epsilon)G_\epsilon(\mathbf{r};\ \mathbf{r}')=-\delta(\mathbf{r}-\mathbf{r}'), \tag{IV.5}$$

where H_0 operates either on $\mathbf{r}$ or on $\mathbf{r}'$. For $\mathbf{r}\neq\mathbf{r}'$, $G_\epsilon(\mathbf{r};\ \mathbf{r}')$ thus satisfies the corresponding homogeneous equation with the boundary condition of being regular at either $\mathbf{r}=0$ or $\mathbf{r}'=0$. These two properties hold as well *for each separate term* of Eq. (IV.4), $G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')$.

(ii) Because the principal value integration in Eq. (IV.2) excludes contributions "on the energy shell," the second term on the right-hand side of Eq. (IV.1) represents a function which is *linearly independent* of all $\mathscr{R}$ functions with energy ϵ. At the same time, this term is a solution of H_0 in the external region corresponding to the *same* eigenvalue ϵ.

Therefore, in analogy with Eq. (IV.3), we can represent the symmetry-adapted principal-value Green's function $G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')$, *for* $\mathbf{r}$ *in the external region and* $\mathbf{r}'$ *in the internal region*, as

$$G^{(\Gamma i)}_\epsilon(\mathbf{r};\ \mathbf{r}')=\pi\sum_{|\mu|_\epsilon}\sum_{Lq}\mathscr{I}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r}';\ \epsilon_\mu). \tag{IV.6}$$

This expansion *defines* the set of *irregular multipole wavefunctions* $\mathscr{I}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)$ which are linearly independent of the multipole wavefunctions $\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)$, which have the same energy ϵ but are constrained to be regular. The actual construction of this set will be discussed below.

Substitution of Eq. (IV.6) into Eq. (IV.1) expresses the elementary solutions, for $\mathbf{r}$ in the external region, as

$$\tilde{\mathscr{R}}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)=\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)+\pi\sum_{|\mu'|_\epsilon}\sum_{Lq'}\mathscr{I}^{(\Gamma i)}_{Lq'}(\mathbf{r};\ \epsilon_{\mu'})\times\langle Lq',\epsilon_\mu|K|Lq,\epsilon_\mu\rangle^{(\Gamma i)}. \tag{IV.7}$$

The corresponding formula for the general solution (III.7) is then

$$\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r}) = \sum_{|\mu|} \sum_{Lq} [\mathscr{R}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)$$

$$+\mathscr{I}^{(\Gamma i)}_{Lq}(\mathbf{r};\ \epsilon_\mu)\beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)] \qquad \text{(IV.8)}$$

with the β's defined in Eq. (III.10). This expression generalizes to a crystal field the familiar expression of the wavefunction outside the range of a spherically symmetric scatterer, as a linear superposition of regular and irregular solutions of the residual Hamiltonian H_0. Note how the dependence on the perturbing potential V is now included in the coefficients β.

The actual construction of the irregular functions $\mathscr{I}$ from the defining equations (IV.2) and (IV.6) requires us to disentangle them from the infinite sum over L in Eq. (IV.6). To this end, notice that, because the $\mathscr{R}$ functions of $\mathbf{r}'$ in the internal region converge to zero as $L\to\infty$, they are not all linearly independent within this region. As a *measure of linear independence* we consider the Gram determinant of the N $\mathscr{R}$ functions with lowest values of L.[18] The value of this determinant decreases steadily as a function of increasing N for large N. Consider a value of N, $N_{\max}$, at which the Gram determinant has fallen below a preestablished low level. The value of L, $L_{\max}$, corresponding to $N_{\max}$ limits a subset of $\mathscr{R}$ functions with $L\leqslant L_{\max}$. We can then construct a set of functions "reciprocal" (i.e., orthogonalized) to this subset of $\mathscr{R}$ functions over the internal region.[19] Successive integration over the internal region of the product of Eqs. (IV.2), or (IV.6), and of each reciprocal function will thus furnish each of the irregular functions $\mathscr{I}$ with $L\leqslant L_{\max}$. Only this subset of $\mathscr{I}_{Lq}$ is, in fact, required in Eq. (IV.8) because the coefficients β_{Lq} vanish for large L. An alternative procedure will be found appropriate for our boundary problem, in Sec. VI, because only the value of $\mathscr{I}$ and of its normal derivative on the boundary are actually needed.

V. THE HARMONICS OF THE BOUNDARY

The coefficients α and β of Eq. (IV.8) must be chosen to satisfy the boundary conditions of continuity of the wavefunction and of its normal derivative *across the boundary* Σ of the internal region. Σ can be the boundary surface of the Wigner–Seitz unit cell containing the impurity, or, more generally, of a number of these cells; that is, Σ is a piecewise smooth surface, consisting of a finite number of plane surfaces. As discussed in the Introduction, we confine the actual matching to the portion of Σ within a single basic domain, because Σ possesses the point group symmetry of the crystal and because the wavefunctions in both the internal and the external region are classified according to symmetry.

We shall perform the matching by expanding the wavefunction and its normal derivative on both side of Σ into *a complete and orthonormal set of harmonics of the boundary surface*. In other words, we shall perform the matching by the method of least squares rather than at a chosen mesh of points over Σ. The harmonics of the boundary surface can be determined by a procedure analogous to that employed in Refs. 2 and 3 to calculate the harmonics of the constant-energy surface in k-space. We then indicate the harmonics of Σ by $Q^{(\Gamma i)}_{\mathscr{L}_q}(\mathbf{r};\ \Sigma)$, the discrete indices $\mathscr{L}_q$ being analogs of the Lq of Refs. 2 and 3. The Q's are:

(i) *orthonormalized* with unit weight over Σ, that is,

$$\oint_\Sigma d\sigma\ Q^{(\Gamma i)}_{\mathscr{L}_q}(\mathbf{r};\ \Sigma)\,Q^{(\Gamma i)}_{\mathscr{L}'_{q'}}(\mathbf{r};\ \Sigma)=\delta_{\mathscr{L}\mathscr{L}'}\,\delta_{qq'}; \qquad \text{(V.1)}$$

(ii) *complete* over Σ, that is, any piecewise smooth function $f^{(\Gamma i)}(\mathbf{r})$ can be expressed *over* Σ as

$$f^{(\Gamma i)}(\mathbf{r})|_\Sigma = \sum_{\mathscr{L}_q} Q^{(\Gamma i)}_{\mathscr{L}_q}(\mathbf{r};\ \Sigma) f^{(\Gamma i)}_{\mathscr{L}_q}, \qquad \text{(V.2)}$$

the coefficients $f^{(\Gamma i)}_{\mathscr{L}_q}$ being determined as usual by

$$f^{(\Gamma i)}_{\mathscr{L}_q} \equiv \langle \mathscr{L}_q | f\rangle^{(\Gamma i)}_\Sigma = \oint_\Sigma d\sigma\, Q^{(\Gamma i)}_{\mathscr{L}_q}(\mathbf{r};\ \Sigma) f^{(\Gamma i)}(\mathbf{r}). \qquad \text{(V.3)}$$

Consider, e.g., the surface of an fcc Wigner–Seitz unit cell. The portion of Σ within the basic domain $(2b\geqslant y\geqslant x\geqslant z\geqslant 0)$ has equation $x+y=2b$ with $b=a/4$, a being the lattice constant. The integral over Σ of any group invariant function then reduces to

$$\oint_\Sigma d\sigma f(x,y,z)=48\sqrt{2}\int_0^b d\eta \int_0^{b-\eta} dz f(b-\eta,\ b+\eta,z) \qquad \text{(V.4)}$$

The overlap integrals entering the expansion of the Q into polynomials in x, y, and z [2,3] can be now calculated anaytically in a lengthy but straightforward way. For stance, $Q_2^{(A_1)}(\mathbf{r};\ \Sigma)$ is proportional to $(r/b)^2-5/2$.

VI. THE MATCHING TO AN IMPURITY

In this section we sketch two alternative methods for calculating the impurity wavefunctions in the internal region and for matching them to the wavefunctions (IV.8) of the external region. Since every energy eigenvalue in the continuum possesses an infinite multiplicity, each method involves boundary conditions that identity a set of solutions uniquely.

A. Outward integration of the Schrödinger equation

Following Altmann *et al.*,[9] one may expand both the centrosymmetric impurity potential and the impurity wavefunctions in the internal region into spherical harmonics symmetry-adapted to the crystal point group about $\mathbf{r}=0$. The Schrödinger equation (III.1) thus reduces to a system of coupled differential equations for the radial wavefunctions. This systems is integrated from $\mathbf{r}=0$ up to the surface of a sphere circumscribing the internal region. Each solution, λ, is identified by initial conditions at $\mathbf{r}=0$. This procedure specifies the values of $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ and of $(\partial/\partial\nu)\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ on the inner face of Σ for each λ. The eigensolutions can be then continued into the surrounding unperturbed crystalline medium by Eq. (IV.8) with coefficients α and β so adjusted that the values of $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ and $(\partial/\partial\nu)\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ coincide on the outer and inner faces of Σ.

The problem of finding the coefficients α and β can be

reduced to an inhomogeneous system of algebraic equations by expanding $\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ and $(\partial/\partial\nu)\Psi^{(\Gamma i)}_{\epsilon,\lambda}(\mathbf{r})$ on both faces of Σ into the harmonics $Q^{(\Gamma i)}_{\mathscr{L}q}(\mathbf{r};\Sigma)$ introduced in Sec. V. With the notation of Eq. (V.3), the system reads

$$\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}\langle\mathscr{L}q|\Psi^{\text{int}}_{\epsilon,\lambda}\rangle^{(\Gamma i)}_{\Sigma}$$
$$=\sum_{\{\mu\}_\epsilon}\sum_{Lq}[\langle\mathscr{L}q|\mathscr{R}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)$$
$$+\langle\mathscr{L}q|\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}\beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\,], \tag{VI.1}$$

and[20]

$$\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}\left\langle\mathscr{L}q\left|\frac{\partial}{\partial\nu}\Psi^{\text{int}}_{\epsilon,\lambda}\right.\right\rangle^{(\Gamma i)}_{\Sigma}$$
$$=\sum_{\{\mu\}_\epsilon}\sum_{Lq}\left[\left\langle\mathscr{L}q\left|\frac{\partial}{\partial\nu}\mathscr{R}_{Lq}(\epsilon_\mu)\right.\right\rangle^{(\Gamma i)}_{\Sigma}\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\right.$$
$$\left.+\left\langle\mathscr{L}q\left|\frac{\partial}{\partial\nu}\mathscr{I}_{Lq}(\epsilon_\mu)\right.\right\rangle^{(\Gamma i)}_{\Sigma}\beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\right]. \tag{VI.2}$$

The normalization factor $\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}$ of the wavefunctions $\Psi^{\text{int}}_{\epsilon,\lambda}$ will be determined by the requirement that the α's and β's satsify Eqs. (III.9) and (III.11).

In Eqs. (VI.1) and (VI.2) the indices $\mathscr{L}$ and L range in principle over an infinite set of values. However, truncation of the sums on the right-hand side to include only the first N terms with lowest L can be guided by the discussion at the end of Sec. IV. Each equation then contains $2N$ unknowns, that is, the $2N$ ratios $\alpha/\mathcal{N}$ and $\beta/\mathcal{N}$. These $2N$ ratios are determined uniquely by Eqs. (VI.1) and (VI.2) by including exactly N terms in the expansions into Q's. Alternatively one might include a larger number of Q's and obtain an approximation for the α's and β's by least squares.[21] Knowledge of N solutions $(\boldsymbol{\alpha}_\lambda, \boldsymbol{\beta}_\lambda)$ $(\lambda=1,...,N)$ is equivalent to calculating the $N\times N$ submatrix of K, Eq. (III.10), "on the energy shell." These N solutions should, in general, be orthonormalized to satisfy Eq. (III.11).

The overlap integrals $\langle\mathscr{L}q|\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}$ and $\langle\mathscr{L}q|(\partial/\partial\nu)\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}$ are to be determined by projecting Eqs. (IV.2) and (IV.6) onto the boundary Σ. In view of the singularities of the Green's function at $\mathbf{r}=\mathbf{r}'$, one may consider initially two slightly separate surfaces, $\Sigma_<$ for $\mathbf{r}'$ and $\Sigma_>$ for $\mathbf{r}$, which then converge onto Σ. Projection onto a pair of harmonics of these surfaces, $Q^{(\Gamma i)}_{\mathscr{L}q}(\mathbf{r};\Sigma_>)$ and $Q^{(\Gamma i)}_{\mathscr{L}'q'}(\mathbf{r}';\Sigma_<)$, gives

$$\sum_\mu \mathscr{P}\int_{\min(E_\mu)}^{\max(E_\mu)}dE$$
$$\times\sum_{Lq}\langle\mathscr{L}q|\mathscr{R}_{Lq}(E_\mu)\rangle^{(\Gamma i)}_{\Sigma}\frac{1}{\epsilon-E}\langle\mathscr{R}_{Lq}(E_\mu)|\mathscr{L}'q'\rangle^{(\Gamma i)}_{\Sigma}$$
$$=\pi\sum_{\{\mu\}_\epsilon}\sum_{Lq}\langle\mathscr{L}q|\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}\langle\mathscr{R}_{Lq}(\epsilon_\mu)|\mathscr{L}'q'\rangle^{(\Gamma i)}_{\Sigma}. \tag{VI.3}$$

As the left-hand side of Eq. (VI.3) is finite, the series on the right-hand side may be truncated after the first N terms. Considering also N harmonics Q only, Eq. (VI.3) reduces to N inhomogeneous systems, each of N equations, for the N^2 unknown matrix elements $\langle\mathscr{L}q|\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}$, which can thus be determined uniquely. One can proceed similarly to determine $\langle\mathscr{L}q|(\partial/\partial\nu)\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}$, noting that the surface integrals remain finite in spite of the sharper singularity of the gradient of the Green's function.

B. Variational calculation within the internal region

A variational method can be used alternatively to calculate the impurity wavefunction within the internal region. In fact, variational methods are particularly suited to deal with nonseparable Schrödinger equations.

For our continuous spectrum where the energy eigenvalue ϵ is specified in advance within the allowed range of a band, we look for the extrema of the integral[22]

$$J[\Psi]=\int_v d\mathbf{r}[(\nabla\Psi)^2+(V_c+V-\epsilon)\Psi^2\,], \tag{VI.4}$$

with the subsidiary condition:

$$\oint_\Sigma d\sigma\,\Psi^2=1. \tag{VI.5}$$

Here V_c+V represents the sum of the unperturbed crystal potential and of the impurity effect, and v and Σ stand for the volume and the surface of the internal region. A necessary condition for an extremum of $J[\Psi]$ is that Ψ satisfies the Schrödinger equation (III.1) with the natural boundary condition

$$\left[\frac{\partial\Psi}{\partial\nu}-b\Psi\right]_\Sigma=0. \tag{VI.6}$$

The constant parameter $b=b_\lambda$ plays the role of eigenvalue of the normal derivative.[22] At any given energy ϵ, the set of boundary values of the corresponding eigenfunctions Ψ_λ is then complete and orthonormal *over* the boundary surface,

$$\oint_\Sigma d\sigma\;\Psi_\lambda\Psi_{\lambda'}=\delta_{\lambda\lambda'}. \tag{VI.7}$$

The matching to the wavefunction in the external region, Eq. (IV.8), can proceed in analogy to Sec. VI A. The boundary values of the variational eigenfunctions Ψ_λ may serve here as the harmonics of the boundary surface. Equations (VI.1) and (VI.2) thus become

$$\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}\delta_{\lambda\lambda'}=\sum_{\{\mu\}_\epsilon}\sum_{Lq}[\langle\lambda'|\mathscr{R}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)$$
$$+\langle\lambda'|\mathscr{I}_{Lq}(\epsilon_\mu)\rangle^{(\Gamma i)}_{\Sigma}\beta_{Lq,\lambda}(\epsilon_\mu)\,], \tag{VI.8}$$

$$\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}b_\lambda\delta_{\lambda\lambda'}$$
$$=\sum_{\{\mu\}_\epsilon}\sum_{Lq}\left[\left\langle\lambda'\left|\frac{\partial}{\partial\nu}\mathscr{R}_{Lq}(\epsilon_\mu)\right.\right\rangle^{(\Gamma i)}_{\Sigma}\alpha^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\right.$$
$$\left.+\left\langle\lambda'\left|\frac{\partial}{\partial\nu}\mathscr{I}_{Lq}(\epsilon_\mu)\right.\right\rangle^{(\Gamma i)}_{\Sigma}\beta^{(\Gamma i)}_{Lq,\lambda}(\epsilon_\mu)\right], \tag{VI.9}$$

where the matrices on the left-hand side of Eqs. (VI.1) and (VI.2) are replaced by $\delta_{\lambda\lambda'}$ and by $b_\lambda \delta_{\lambda\lambda'}$.

The alternative methods of Secs. VI A and VI B might complement each other in practical calculations. For example, the outward integration method might provide a set of N functions at a coarse mesh of values of ϵ. These functions might, in turn, be used as trial functions for a Rayleigh–Ritz variational calculation at a finer mesh of ϵ.

VII. DISCUSSION

Photoabsorption cross sections have been generally obtained as products of squared dipole matrix elements and of the density of states. It has been increasingly recognized[23] that the density of states should be apportioned among channels of different symmetries and should reflect local impurity effects for each channel. The allotment of the "local" density of states among the various channels was considered earlier in Ref. 2. Here we have identified the relevant density as the square of the normalization factor $\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}$ of Sec. VI, with the understanding that the matrix element is calculated with the internal final state function $\Psi^{\rm int}_{\epsilon,\lambda}$. This normalization factor incorporates the effects of the band structure in the external region. The dependence of $\mathcal{N}^{(\Gamma)}_{\epsilon,\lambda}$ on the energy ϵ will thus modulate the photoabsorption profile by reflecting the influence of the external region on the rate of escape of the photoelectron.

The current EXAFS theories[24] ascribe the modulation of photoabsorption to interference between the wavefunction of the escaping electron and the waves backscattered by the surrounding crystal structure. In our approach the effects of these reflections are incorporated in the conditions over the boundary of the internal region; thereby, multiple scatterings are taken into account to all orders because the wavefunction in the external region takes full account of the crystal field. Our approach is thus particularly suited to energies close to the threshold, while the EXAFS is suited to escape energies $\gtrsim$ 30–50 eV.

The formalism of this paper can also be applied to the calculation of scattering processes in crystals since Eq. (III.10) provides the K matrix on the energy shell.

Our approach should eventually be extended to include a many-particle treatment of the internal region. This could be done, in analogy with atomic calculations,[25] by a many-body variational procedure which would also have to take into account the relaxation of the medium around the hole. A detailed procedure for this purpose remains, however, to be developed.

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Neutrino fields in axially and reflection symmetric space-times[a)]

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It is shown that there exist no physically significant (i.e., nonsingular) solutions to the Einstein-neutrino field equations in an axially and reflection symmetric space-time.

I. INTRODUCTION

Solutions of the Einstein-neutrino (E-n) field equations are interesting for, at least, three reasons:

(1) It has long been believed, specially since the discovery of the neutral currents, that the neutrino transport mechanism plays a crucial role in the supernovae evolution.[1]

(2) The E-n equations allow the existence of neutrinos whose energy–momentum tensor vanishes identically but whose current vector does not ("ghost neutrinos).[2-6]

(3) Under certains conditions (e.g., spherical symmetry, axial symmetry and nongravitational radiation, etc.) the E-n equations have no solution at all, not even "ghost" solutions.[7-11]

We started our research motivated by point (1): specifically, we were looking for a model of a star simultaneously emitting neutrinos and gravitational waves under certains symmetric restrictions. At the end, due to our results, we focused our attention on point (2) and specifically on (3).

In the present paper we shall consider an axially and reflection symmetric space–time which is asymptotic flat, without any further conditions on the gravitational field (i.e., it can be radiative, nonradiative and time dependent, or static) we shall solve the E-n field equations and show that the energy–momentum tensor of the neutrino field vanishes identically and the neutrino flux vector contains a singularity.

We are going to use the formalism of Bondi *et al.*,[12] a short description of which is given in Sec. II.

In the third section the equations of the E-n field will be explicitly written following a paper by Griffiths and Newing.[13] The energy–momentum tensor of the neutrino field as well as the neutrino flux vector is found.

At the end some comments and remarks are included in the conclusion.

II. BONDI'S FORMALISM

The general form of an axially symmetric asymptotically flat metric given by Bondi is[12]

$$ds^2=(Vr^{-1}e^{2\beta}-U^2r^2e^{2\gamma})\,du^2+2e^{2\beta}\,du\,dr$$
$$+2Ur^2e^{2\gamma}\,du\,d\theta-r^2(e^{2\gamma}\,d\theta^2+e^{2\gamma}\sin^2\theta\,d\phi^2), \quad (1)$$

the four functions U, β, γ, V, are functions of u, r, and θ, where $x^0=u$ is a timelike coordinate, $x^1\equiv r$ a null radial coordinate, $x^2\equiv\theta$ an angular coordinate, and $x^3\equiv\phi$ the axial rotation angle.

An examination of the Bianchi identities shows the Einstein equations

$$G_{\alpha\beta}\equiv R_{\alpha\beta}+E_{\alpha\beta}=0$$

split into three groups:

(i) four main equations

$$G_{11}=0, \quad (2)$$
$$G_{12}=0, \quad (3)$$
$$G_{22}=0, \quad (4)$$
$$G_{33}=0, \quad (5)$$

(ii) two supplementary conditions

$$G_{00}=0, \quad (6)$$
$$G_{02}=0, \quad (7)$$

(iii) and one trivial equation

$$G_{01}=0.$$

The four metric functions are assumed to be expanded in power series of $1/r$; using the main equations, Bondi obtains for the vacuum case ($E_{\alpha\beta}=0$)

$$\gamma=c(u,\theta)r^{-1}+[C(u,\theta)-\tfrac{1}{6}c^3]r^{-3}+\cdots, \quad (8)$$

$$U=-(c_\theta+2c\cot\theta)r^{-2}+[2N(u,\theta)$$
$$+3cc_\theta+4c^2\cot\theta]r^{-3}+\cdots, \quad (9)$$

$$V=r-2M(u,\theta)-[N_\theta+N\cot\theta-c^2_\theta$$
$$-4cc_\theta\cot\theta-\tfrac{1}{2}c^2(1+8\cot^2\theta)r^{-1}+\cdots, \quad (10)$$

$$\beta=-\tfrac{1}{4}c^2r^{-2}+O(r^{-4}), \quad (11)$$

and

$$4C_u=2c^2c_u+2cM+N\cot\theta-N_2, \quad (12)$$

where c, N, and M appear as functions of integrations. At this point it is shown by Bondi *et al.* that, given γ for one value of u and given the three functions $c(u,\theta)$, $N(u,\theta)$, and

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$M(u,\theta)$, the entire development is determined by the four main equations.

Next, in the two supplementary conditions (6), (7) only the inverse square term survives, an involve only relations between the three functions c, M, N and the inverse square law term of E_{02} and E_{00}

$$r^2G_{00}=2M_{,u}+2c_{,u}^2-(c_{,\theta\theta}+3c_{,\theta}\cot\theta-2c)_{,u}+E_{00}^{(2)}=0, \tag{6'}$$

$$r^2G_{02}=-3N_{,u}-M_{,\theta}-3cc_{,u\theta}+4cc_{,u}\cot\theta-c_{,u}c_{,\theta}+E_{02}^{(2)}=0. \tag{7'}$$

We shall use letters as subscripts to denote derivatives; for example

$$f_{,\theta}=\frac{\partial f}{\partial\theta}=\partial_{,\theta}f=f,\theta.$$

Superscripts will be used to denote the coefficients of each power for example

$$f=f^{(-N)}r^n+\cdots+f^{(-1)}r+f^{(0)}+f^{(1)}r^{-1}+\cdots.$$

III. EINSTEIN-NEUTRINO FIELD

A given space–time will admit a neutrino field if a null tetrad can be constructed satisfying the equations[13]

$$K^{\nu}{}_{;\nu}=0, \tag{13}$$

$$(K_{\mu}t^{\nu}-t_{\mu}K^{\nu})_{;\nu}=t^{\alpha}K_{\alpha;\mu}, \tag{14}$$

$$R_{\mu\nu}+E_{\mu\nu}=0, \tag{15}$$

$$E_{\mu\nu}=i(H_{\mu}\bar{t}_{\nu}+H_{\nu}\bar{t}_{\mu}-\bar{H}_{\mu}t_{\nu}-\bar{H}_{\nu}t_{\mu}+P_{\mu}K_{\nu}+P_{\nu}K_{\mu}) \tag{16}$$

(bars mean complex conjugation), where

$$H_{\mu}=t^{\alpha}K_{\alpha;\mu}, \tag{17}$$

$$P_{\mu}=\bar{t}^{\alpha}t_{\alpha;\mu}, \tag{18}$$

and the tetrad vectors $(K,m,t,\bar{t})$ satisfy the following conditions:

$$\begin{aligned}&m^{\alpha}K_{\alpha}=-t^{\alpha}\bar{t}_{\alpha}=1,\\&m^{\alpha}m_{\alpha}=K^{\alpha}K_{\alpha}=t^{\alpha}t_{\alpha}=m^{\alpha}t_{\alpha}=k^{\alpha}t_{\alpha}=0,\\&g^{\alpha\beta}=m^{\beta}K^{\alpha}+m^{\alpha}k^{\beta}-\bar{t}^{\alpha}t^{\beta}-t^{\alpha}\bar{t}^{\beta}.\end{aligned} \tag{19}$$

The vector K_{ν} is interpreted as the neutrino flux vector [see Eq. (13)]. Equations (14) are the Weyl's equations for the two component neutrino in terms of the tetrad. The energy–momentum tensor for the neutrino field is given by (16).

Let us start by choosing a tetrad satisfying the conditions (19). One such tetrad could be[14]

$$K^{\alpha}(0,e^{-2\beta},0,0), \tag{20}$$

$$m^{\alpha}(1,-\tfrac{1}{2}Vr^{-1},U,0), \tag{21}$$

$$t^{\alpha}(0,0,\tfrac{1}{2}r^{-1}e^{-\gamma}(1+i),\tfrac{1}{2}(1-i)e^{\gamma}r^{-1}\sin^{-1}\theta). \tag{22}$$

In order to satisfy Eq. (13), we apply a boost in the (K,m) plane, obtaining a new tetrad:

$$K'_{\mu}=A^{-1}K_{\mu},$$

$$m'_{\mu}=Am_{\mu},$$

$$t'_{\mu}=t_{\mu},$$

and choosing the boost parameter A, so that

$$K'^{\nu}{}_{;\nu}=0.$$

A very simple calculation gives $A=f(u,\theta)r^2$, where $f(\theta,u)$ is an arbitrary function

Hence, the appropriate tetrad is (we omit the primes)

$$K^{\alpha}(0,A^{-1}e^{-2\beta},0,0), \tag{23}$$

$$m^{\alpha}(A,-\tfrac{1}{2}AVr^{-1},AU,0), \tag{24}$$

$$t^{\alpha}(0,0,\tfrac{1}{2}r^{-1}e^{-\gamma}(1+i),\tfrac{1}{2}(1-i)e^{\gamma}r^{-1}\sin^{-1}\theta), \tag{25}$$

the covariant components being

$$K_{\alpha}(A^{-1},0,0,0),$$

$$m_{\alpha}(\tfrac{1}{2}AVr^{-1}e^{2\beta},Ae^{2\beta},0,0),$$

$$t_{\alpha}(Ure^{\gamma}(1+i)\tfrac{1}{2},0,-\tfrac{1}{2}re^{\gamma}(1+i),-\tfrac{1}{2}(1-i)re^{-\gamma}\sin\theta).$$

For practical purposes, it is better to work out the calculations in terms of the spin coefficients[15]

$$\begin{aligned}&\kappa=K_{\mu;\nu}t^{\mu}K^{\nu}, && \nu=-m_{\mu;\nu}\bar{t}^{\mu}m^{\nu},\\&\rho=K_{\mu;\nu}t^{\mu}\bar{t}^{\nu}, && \mu=-m_{\mu;\nu}\bar{t}^{\mu}t^{\nu},\\&\sigma=K_{\mu;\nu}t^{\mu}t^{\nu}, && \lambda=-m_{\mu;\nu}\bar{t}^{\mu}\bar{t}^{\nu},\\&\tau=K_{\mu;\nu}t^{\mu}m^{\nu}, && \Pi=-m_{\mu;\nu}\bar{t}^{\mu}K^{\nu},\\&\alpha=\tfrac{1}{2}(K_{\mu;\nu}m^{\mu}\bar{t}^{\nu}-t_{\mu;\nu}\bar{t}^{\mu}\bar{t}^{\nu}),\\&g=\tfrac{1}{2}(K_{\mu;\nu}m^{\mu}t^{\nu}-t_{\mu;\nu}\bar{t}^{\mu}m^{\nu}),\\&\epsilon=\tfrac{1}{2}(K_{\mu;\nu}m^{\mu}K^{\nu}-t_{\mu;\nu}\bar{t}^{\mu}K^{\nu}),\\&b=\tfrac{1}{2}(K_{\mu;\nu}m^{\mu}t^{\nu}-t_{\mu;\nu}\bar{t}^{\mu}t^{\nu})\end{aligned}$$

(the spin coefficients g and b are usually denoted by γ and β respectively; we use Latin letters to avoid confusion with the metric functions γ and β).

Using (19), we can write

$$\begin{aligned}t_{\mu;\nu}=&-\kappa m_{\mu}m_{\nu}-\tau m_{\mu}K_{\nu}+\sigma m_{\mu}\bar{t}_{\nu}+\rho m_{\mu}t_{\nu}\\&+K_{\mu}m_{\nu}\bar{\Pi}\bar{\nu}K_{\mu}K_{\nu}-\bar{\lambda}K_{\mu}\bar{t}_{\nu}-\bar{\mu}K_{\mu}t_{\nu}\\&-t_{\mu}t_{\nu}(\bar{\epsilon}-\epsilon)-t_{\mu}K_{\nu}(\bar{g}-g)\\&+t_{\mu}\bar{t}_{\nu}(\bar{\alpha}-b)+(\bar{b}-\alpha)t_{\mu}t_{\nu},\end{aligned} \tag{26}$$

$$\begin{aligned}K_{\mu;\nu}=&(g+\bar{g})K_{\mu}K_{\nu}+(\epsilon+\bar{\epsilon})K_{\mu}m_{\nu}+(\alpha+\bar{b})K_{\mu}t_{\nu}\\&-(\bar{\alpha}+b)K_{\mu}\bar{t}_{\nu}-\bar{\tau}t_{\mu}K_{\nu}-\tau\bar{t}_{\mu}K_{\nu}\\&-\bar{\kappa}t_{\mu}m_{\nu}-\kappa\bar{t}_{\mu}m_{\nu}\\&+\bar{\sigma}t_{\mu}t_{\nu}+\sigma\bar{t}_{\mu}\bar{t}_{\nu}+\bar{\rho}t_{\mu}\bar{t}_{\nu}+\rho\bar{t}_{\mu}t_{\nu};\end{aligned} \tag{27}$$

therefore, Eq. (13) becomes

$$\epsilon+\bar{\epsilon}=\bar{\rho}+\rho. \tag{28}$$

Multiplying Eqs. (14) by K^{α}, m^{α}, t^{α}, and $\bar{t}^{\alpha}$ successively and using (26), (27), one gets respectively

$$\kappa=\kappa, \tag{29}$$

$$b=\tau, \tag{30}$$

$$\sigma=\sigma, \tag{31}$$

$$\epsilon-\bar{\epsilon}=\bar{\rho}-\rho. \tag{32}$$

Thus Eqs. (13) and (14) are equivalent to

$$\epsilon=\rho, \tag{33}$$

$$b=\tau. \tag{34}$$

For the energy–momentum tensor (16) one finds without difficulty the equivalent expression

$$\begin{aligned} E_{\mu\nu}=&2i\{(\bar{g}-g)K_{\mu}K_{\nu}+(\bar{\epsilon}-\epsilon)[K_{(\mu}m_{\nu)}+t_{(\mu}\bar{t}_{\nu)}] \\ &-(2\bar{b}-\alpha)K_{(\mu}t_{\nu)}+(2b-\bar{\alpha})K_{(\mu}\bar{t}_{\nu)} \\ &-2i\sigma\bar{t}_{\mu}\bar{t}_{\nu}+\bar{\sigma}t_{\mu}t_{\nu}+km_{(\mu}\bar{t}_{\nu)} \\ &--km_{(\mu}t_{\nu)}\}. \end{aligned} \tag{35}$$

Let us now calculate the explicit form of the spin coefficients in terms of our tetrad field. A straightforward calculation gives

$$\kappa=0,$$

$$\epsilon=-e^{-2\beta}A^{-1}r^{-1}, \tag{36}$$

$$\rho=-A^{-1}e^{-2\beta}r^{-1},$$

$$\tau=-\tfrac{1}{2}e^{-\gamma}(1+i)\times[r^{-1}\beta_{\theta}-re^{2(\gamma-\beta)}(\tfrac{1}{2}U_{r}+\gamma_{r}U)+Ue^{2(\gamma-\beta)}r\gamma_{r}],$$

$$\begin{aligned} b=&-\tfrac{1}{2}e^{-\gamma}(1+i)\{\tfrac{1}{2}r^{-1}[f^{-1}\partial_{\theta}f+\beta_{\theta}(-r^2/2)e^{2(\alpha-\beta)}U_{r}] \\ &+\tfrac{1}{4}Ue^{2\gamma}(e^{2\beta}-e^{-2\beta})+\tfrac{1}{4}r^{-1}\gamma_{\theta}-\tfrac{1}{4}r^{-1}\cot\theta\}, \end{aligned} \tag{37}$$

$$\begin{aligned} \alpha=&[(1-i)/4r]e^{-\gamma}[r^2e^{2(\gamma-\beta)}U_{r} \\ &-(1/f)(f_{u}+2f\beta_{u})-r^2(f_{\theta}+2f\beta_{\theta})], \end{aligned}$$

$$\begin{aligned} \gamma=&\tfrac{1}{4}f(V+rV_{r}+2rV\beta_{r})-(1/f)(f_{u}-2f\beta_{u}) \\ &-Ur^2(f_{\theta}+2f\beta_{\theta}) \end{aligned}$$

$$\sigma=(-i/2fr^2)e^{-2\beta}\gamma_{r}.$$

One can see at once that Eq. (33) is automatically satisfied. Equation (34) will be discussed later.

Let us now come back to the field equations, with the help of (36) and (35) one gets

$$E_{11}=0,\ E_{12}=0,\ E_{33}=0,\ E_{22}=0.$$

Thus the main equations (2)–(5) and consequently the expressions (8)–(12) are the same as in the vacuum case. Next, since the two supplementary conditions (6), (7) are reduced to the inverse-square-law term, we only need $E^{(2)}_{02}$ and $E^{(2)}_{00}$. A simple calculation gives

$$E^{(2)}_{00}=E^{(2)}_{02}=0,$$

The other components of the energy–momentum tensor vanishes because of the symmetry of the problem.

So far we have seen that any possible solution of the E-n equations, under our conditions must be a "ghost" solution. Let us now return to Eq. (34) and see if these solutions can exist at all. Feeding back the expressions (8)–(12) into (34), we get, for the order $O(r^{-1})$,

$$f^{-1}\partial_{2}f=\tfrac{1}{2}\cot\theta, \tag{38}$$

for the order $O(r^{-2})$

$$c=0, \tag{39}$$

for the order $O(r^{-3})$

$$N=0, \tag{40}$$

for the order $O(r^{-4})$

$$C=\sin\theta^{-12/7}\cdot\Psi(u); \tag{41}$$

since angular singularities are not allowed in the metric, we get

$$C=0. \tag{42}$$

Expressions (39), (40), and (42) imply a spherical symmetric metric, and Eq. (38) gives

$$f=\phi(u)\sin\theta^{1/2},$$

$\phi(u)$ being an arbitrary function of u. The final expression for the neutrino flux vector is thereby singular in the axis $\theta=(0,\pi)$,

$$K_{\nu}(\phi^{-1}(u)\ \sin\theta^{-1/2}r^{-2},0,0,0). \tag{43}$$

IV. CONCLUSION

The results of this paper suggests that the Einstein-neutrino system is specially sensible to symmetric restrictions. The next step should be to find out which, if any, of the three restrictions, axial symmetry, reflection symmetric, and asymptotic flatness, is by itself responsible for the situation and furthermore if there is any relationship between the symmetry restriction and some specific properties of the neutrino. This last point leads us to a more fundamental question concerning the physical meaning of the classical results for Fermi fields.

In fact, it is well known that the classical neutrino theory is not without its problems.[16,17] One major problem being the abscence, In the classical approach, of the Pauli exclusion principle.

It should be realized that the relevance of any solution of the E-n equations depends on the answer to the last question.

Finally we would like to remark that, though the series expansions (8)–(11) are not in general valid starting with certain term in the development, the results we have obtained just require the first term in (8) to be true. We recall that this is essentially equivalent to Sommerfeld's radiation condition.

To obtain (39), (40) and (42), higher orders in the expansion (8)–(11) are required. But the information this equation gives [together with (38)] is that the neutrino flux vector in a spherical symmetric metric is singular. This is a known result,[8,11] so that the expansion up to required orders, in this case, seems to be justified.

We would like to thank the referee for this point and a question concerning the choice of the neutrino flux vector.[14]

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[14]For the null vector K^{α} to be the neutrino flux vector it must be tangent to the outgoing null rays and it must satisfy equation (13).

In our coordinate system the first condition means that

$$K_{\alpha}=F(u,\theta,r)\frac{\partial u}{\partial x^{\alpha}},$$

$$K^{\alpha}=G(u,\theta,r)\frac{\partial x^{\alpha}}{\partial r}.$$

In order to satisfy Eq. (13), we can use the coordinate transformation freedom and the null rotations of the tetrad. We restrict ourselves to transformation which leaves the direction of K^{α} unchanged, namely: (a) Rotation about K^{α}; (b) Boost in the (K,m) plane; (c) $u\to p(u)$, $r\to r/p(u)$. Doing so, we keep the meaning of the vector K^{α} as the neutrino flux vector.

Surely, the set of the transformations which leave invariant the metric (BMS and all the null rotations) is larger than the set of previously mentioned transformations.

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Solutions of the generalized nonlinear Schrödinger equation in two spatial dimensions

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Recently, from two independent methods, the generalized nonlinear Schrödinger evolution equation in two spatial dimensions has been derived both by Ablowitz and Haberman and by Morris. Here the same extension of the Schrödinger cubic equation is obtained from a two-dimensional spatial inversionlike integral equation when a suitable time dependence is introduced. We investigate the solutions (corresponding to degenerate kernels of the inversion equation) in both cases, where the nonlinear part reduces or not to a cubic term. While in the first case, the solutions are not confined, on the contrary in the second case, we show explicitly for any finite time, that there exists an infinite number of solutions which are confined in the two-dimensional coordinate space.

I. INTRODUCTION

The generalization of the nonlinear Schrödinger equation in two spatial dimensions has recently been derived by two different methods: firstly by Ablowitz and Haberman,[1] requiring the compatibility conditions for two linked partial differential systems. Secondly, Morris,[2] generalizing the nice and powerful "prolongation structure" method of Wahlquist and Estabrook[3] in twospatial dimensions, has also obtained[4] the generalized nonlinear Schrödinger equation. However both methods give the extension of the evolution equations but do not provide the explicit construction of the solution and this last point is the aim of the present paper.

Recently[5] we have established an inversionlike integral equation (IE) associated with a partial differential system, from which we can construct both a class of potentials and of solutions. In particular it was shown, in the case where the kernels of the IE depend upon two independent variables, that among the potentials reconstructed from this IE, there exists a family of confined ones in a two-dimensional coordinate space.

In Sec. II, we recall very briefly the results of the IE in the two-dimensional space and establish some general properties useful later for the derivation of the evolution equations.

In Sec. III we introduce the time in the kernels of the IE, assume that they satisfy the two-dimensional spatial heat equation (for imaginary time), and also deduce the generalized nonlinear Schrödinger equation,

$$\left(\frac{i\partial}{\partial t}+\alpha_1\frac{\partial^2}{\partial x_1^2}+\alpha_2\frac{\partial^2}{\partial x_2^2}\right)A+2A\,(\alpha_1 B_{x_1}+\alpha_2 C_{x_2})=0\,,$$

$$B_{x_2}=C_{x_1}=-\eta\,|A|^2,\quad \alpha_i,\ \eta \quad \text{are real,} \tag{1}$$

where A,B,C depend upon three variables x_1, x_2, t, and $B_{x_1}\cdots$ means $\partial B/\partial x_1,\cdots$. Equation (1) with trivial changes of coordinate variables can be compared with the above recalled equations (for instance $x_1 \pm x_2$ with the Morris's equation). The nonlinear part in Eq. (1) reduces to the usual cubic term if the derivatives B_{x_1} and B_{x_2} (as well as C_{x_1} and C_{x_2}) are proportional. This case requires that the modulus of the kernel of the IE depends upon only one variable and so we are able to distinguish both cases where the nonlinear part of (1) is cubic or not.

The most simple degenerate kernel of the IE (the soliton case in one spatial dimension) is obtained by multiplying any solution of the heat equation [linear part of Eq. (1)] corresponding to one coordinate by any solution of the same equation for the other coordinate (of course taking into account boundary conditions). In this manner we exhibit in Sec. IV, for the nonpurely cubic case, an infinite number of solutions of Eq. (1), confined, for any finite time, in the x_1x_2 plane. For instance, one of them is

$$\Phi=\frac{\Pi_{j=1}^{2}(\mu_j)^{-1/2}\exp(x_j^2/\mu_j)}{1-\eta\,\Pi_{j=1}^{2}(\sqrt{|\mathrm{Re}\mu_j|})^{-1}\int_{\tilde{x}_j}^{\infty}dV_j\exp(-2V_j^2)}$$

$$\begin{cases}\mu_j=\eta_j-4i\alpha_j t, & \mathrm{Re}\mu_j=\mathrm{Re}\eta_j<0\\ \tilde{x}_j=x_j\dfrac{\sqrt{|\mathrm{Re}\mu_j|}}{|\mu_j|}\end{cases} \tag{2}$$

Further for the pure cubic nonlinear part of Eq. (1), we have found that the solutions are not confined.

When the kernel of the IE is a finite sum of discrete terms (the multisoliton case in one dimension) we have found similar features for the solutions in both cases.

II. INVERSIONLIKE INTEGRAL EQUATIONS ASSOCIATED WITH A TWO-DIMENSIONAL SYSTEM OF FIRST ORDER LINEAR EQUATIONS

A. The results of Ref. 5

(i) Let us consider for $i=1,2, j=1,2$ the integral equation:

$$K_j^i(x_1,x_2;y)=\tilde{F}_j^i+\sum_{m=1}^{m=2}\int_{x_m}^{\infty}F_m^i K_j^m(x_1,x_2;s)ds\,,$$

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$$F^i_m = F^i_m\{\epsilon^i_m[\lambda_m(x_m - s) + \lambda_i x_i]\eta^i_m;$$
$$\eta^i_m[\lambda_i(x_i - y) + \lambda_m x_m]\},$$
$$(\epsilon^i_m)^2 = (\eta^i_m)^2 = 1, \tag{3}$$
$$\tilde{F}^i_j = F^i_j(s = x_j) = F^i_j\{\epsilon^i_j\lambda_i x_i;\ \eta^i_j[\lambda_i(x_i - y) + \lambda_j x_j]\},$$

where the kernels F^i_j depend upon two independent variables and the λ_i are fixed numbers.

(ii) We assume

$$\lim_{y\to\infty} F^i_j = \lim_{s\to-\infty} F^i_m K^m_j = 0. \tag{4a}$$

We can verify from Eq. (3)

$$\lambda_i^{-1}(F^i_j)_{x_i} = \lambda_j^{-1}(F^i_j)_{x_j} = -\left(\lambda_j^{-1}\frac{\partial}{\partial s} + \lambda_i^{-1}\frac{\partial}{\partial y}\right)F^i_j \tag{5}$$

$$\left(\frac{\partial}{\partial x_j} + \frac{\lambda_j}{\lambda_i}\frac{\partial}{\partial y}\right)K^i_j = K^i_m\hat{K}^m_j\lambda_j\lambda_m^{-1}, \quad m \neq j,$$
$$\hat{K}^m_j = K^m_j(x_1, x_2; y = x_m). \tag{6}$$

(iii) We define two components vector columns constructed from the solutions K^i_j of Eq. (3)

$$\psi_j = \left[U^0_j(x_j)\delta^i_j + \int_{x_j}^{\infty} U^0_j(y)\,K^j_i(x_1, x_2; y)dy\right],$$
$$j = 1,2, \quad i = 1,2, \tag{7}$$
$$\left(\frac{\partial}{\partial x} + i\lambda_j k\right)U^0_j(x) = 0.$$

(iv) If we assume

$$\lim_{y\to\infty} U^0_i(y)\,K^i_j(x_1, x_2;\ y) = 0, \tag{4b}$$

and define

$$q^i_j(x_1, x_2) = \lambda_j(\lambda_i)^{-1}\hat{K}^i_j, \tag{8}$$

Then the ψ_j $(j = 1,2)$ defined in (7) are solutions of the partial differential system

$$\begin{pmatrix} \frac{\partial}{\partial x_1} + i\lambda_1 k & -q^2_1 \\ -q^1_2 & \frac{\partial}{\partial x_2} + i\lambda_2 k \end{pmatrix}\psi_j = 0, \quad j = 1,2. \tag{9}$$

Equation (3) is an inversionlike integral equation giving the possibility of constructing a class of potentials q^1_2, q^2_1 and a class of solutions ψ_1, ψ_2 associated with the system (9), when we introduce into Eq. (3) kernels F^i_j such that the conditions (4a) and (4b) are satisfied.

B. Some properties of the solutions of the (IE) Eq. (3)

We sketch very briefly a set of properties which will be useful in Sec. III for the derivation of the evolution equation (1) associated with Eq. (3). For simplicity, in the remainder of the paper we consider in (3)–(9): $\lambda_1 = \varepsilon^1_2 = \eta^2_1 = 1$, $\lambda_2 = \eta^1_2 = \varepsilon^2_1 = -1$, $F^1_1 = F^2_2 = 0$ such that if we write Eq. (3) in a matrix form:

$$\mathscr{K}(x_1, x_2; y) = \tilde{\mathscr{F}}(x_1, x_2; y) + \int_{-\infty}^{+\infty} \mathscr{F}(x_1, x_2; s; y)\,\mathscr{K}(x_1, x_2; s)\,ds,$$

$$\mathscr{K} = \begin{pmatrix} K^1_1 K^1_2 \\ K^2_1 K^2_2 \end{pmatrix},$$

$$\tilde{\mathscr{F}} = \begin{pmatrix} 0 & \tilde{F}^1_2 = F^1_2(x_1; y - x_1 + x_2) \\ \tilde{F}^2_1 = F^2_1(x_2, y - x_2 + x_1) & 0 \end{pmatrix}, \tag{3'}$$

$$\mathscr{F} = \begin{pmatrix} 0 & F^1_2(s - x_2 + x_1; y - x_1 + x_2)\theta(s - x_2) \\ F^2_1(s - x_1 + x_2; y - x_2 + x_1)\theta(s - x_1) & 0 \end{pmatrix}.$$

1. We define

$$O_{sx_j} = \frac{\partial}{\partial x_j} + \frac{\partial}{\partial y}, \quad O_{dx_j} = \frac{\partial}{\partial x_j} - \frac{\partial}{\partial y}.$$

Equation (6) can be rewritten

$$\begin{pmatrix} O_{sx_1} & K^1_1 & O_{dx_2} & K^1_2 \\ O_{dx_1} & K^2_1 & O_{sx_2} & K^2_2 \end{pmatrix} + \begin{pmatrix} K^1_1 & K^1_2 \\ K^2_1 & K^2_2 \end{pmatrix}\begin{pmatrix} 0 & \hat{K}^1_2 \\ \hat{K}^2_1 & 0 \end{pmatrix} = 0. \tag{6'}$$

In particular, from Eq. (6) we get:

$$\hat{K}^i_{i,x_i} + \hat{K}^i_j\hat{K}^j_i = 0, \quad j \neq i \tag{6a}$$
$$\hat{K}^i_{j,x_j} - \left(\frac{\partial}{\partial y}K^i_j\right)_{y=x_j} + \hat{K}^i_i\hat{K}^i_j = 0, \quad j \neq i, \tag{6b}$$
$$-K^i_i\hat{K}^i_{j,x_j} + K^i_{j,yy} = K^i_{j,x_jx_j} + \hat{K}^i_j O_{sx_j}K^i_i. \tag{6c}$$

2. In the following, by straightforward algebraic calculations, we derive, from Eq. (3), a set of integral equations for

quantities linked to $\mathscr{K}$ (when derivatives with respect to x_1,x_2,y appear). These equations have the same kernel $\mathscr{F}$ as in Eq. (3) but different free terms. We will get relations of the type

$$\mathscr{H}_i(x_1,x_2;y)=\mathscr{H}_i^0(x_1,x_2;y)+\int\mathscr{F}(x_1,x_2;s;y)\,\mathscr{H}_i(x_1,x_2;s)ds\,, \tag{10}$$

where $\mathscr{H}_i$, $\mathscr{H}_i^0$ are 2×2 matrices linked to $\mathscr{K}$, $\mathscr{F}$, $\widetilde{\mathscr{F}}$ and their derivatives,

$$\mathscr{H}_1=\begin{pmatrix} O_{dx_2} & K_1^1 & O_{sx_1} & K_2^1\\ O_{sx_2} & K_1^2 & O_{dx_1} & K_2^2\end{pmatrix},$$

$$\mathscr{H}_1^0=-\mathscr{F}\begin{pmatrix}\widehat{K}_1^1 & 0\\ 0 & \widehat{K}_2^2\end{pmatrix}+\begin{pmatrix}0 & O_{sx_1} & \widetilde{F}_2^1\\ O_{sx_2} & \widetilde{F}_1^2 & 0\end{pmatrix}, \tag{10a}$$

$$\mathscr{H}_2=\begin{pmatrix} O^2_{dx_2} & K_1^1 & O^2_{sx_1} & K_2^1\\ O^2_{sx_2} & K_1^2 & O^2_{dx_1} & K_2^2\end{pmatrix},$$

$$\mathscr{H}_2^{(0)}=-\mathscr{F}\begin{pmatrix}\widehat{K}^1_{1x_2}+(O_{dx_2}K_1^1)_{y=x_1} & 0\\ 0 & \widehat{K}^2_{2x_1}+(O_{dx_1}K_2^2)_{y=x_2}\end{pmatrix}$$

$$+\begin{pmatrix}0 & O^2_{sx_1} & \widetilde{F}_2^1\\ O^2_{sx_2} & \widetilde{F}_1^2 & 0\end{pmatrix}-\begin{pmatrix}0 & O_{sx_1} & \widetilde{F}_2^1\\ O_{sx_2} & \widetilde{F}_1^2 & 0\end{pmatrix}\begin{pmatrix}\widehat{K}_2^2 & 0\\ 0 & \widehat{K}_1^1\end{pmatrix} \tag{10b}$$

3. If we are interested in cases where the potentials $q_j^i=-\widehat{K}_j^i$ are linked, we must find the corresponding relations between the kernels F_2^1 and F_1^2. The two interesting cases are when one potential is proportional either to the other or to the complex conjugate of the other.

Let us remark that in Eq. (3) the equations decouple and we get

$$K_j^i(x_1,x_2;y)$$
$$=F_j^i(x_i;y-x_i+x_j)+\int_{x_j}ds\int_{x_i}du$$
$$\times F_j^i(s-x_j+x_i;y-x_i+x_j)$$
$$\times F_i^j(u-x_i+x_j;s-x_j+x_i)\,K_j^i(x_1,x_2;u)\,,\ i\neq j,$$

$$\widehat{K}_i^i=\int_{x_j}F_j^i(s-x_j+x_i;x_j)\,K_i^j(x_1,x_2;s)ds\,. \tag{11}$$

4. In Appendix A we study both Eq. (11) when $\widehat{K}_1^2=\eta(\widehat{K}_2^1)^*$ and we get the two following properties:

(i) If the F_j^i satisfy

$$F_1^2(u;v)=\eta\,[F_2^1(v;u)\,]^*, \tag{12a}$$

then the $\widehat{K}_j^i$ satisfy

$$\widehat{K}_1^2=\eta(\widehat{K}_2^1)^*,\ \widehat{K}^i_{i,x_i}+\eta|\widehat{K}_2^1|^2=0,\ \widehat{K}_i^i \text{ are real.} \tag{12b}$$

(ii) If either for $i=1$ or $i=2$ we have

$$\widehat{K}^i_{i,x_i}=\xi_i\widehat{K}^i_{i,x_j},F_1^2(u;v)=\eta\,[F_2^1(v;u)\,]^*, \tag{13a}$$

ξ_i being real, then we get for $\widehat{K}_i^i$ and $|F_2^1|$:

$$\widehat{K}_i^i \text{ is a function of } \xi_i x_i+x_j,\ \xi_i\xi_j=1 \tag{13b}$$

$$\left(\frac{\partial}{\partial u}-\xi_1\frac{\partial}{\partial v}\right)|F_2^1(u;v)|=0 \quad\text{or}\quad |F_2^1(u;v)|=|F_2^1(\xi_1u+v)|\,.$$

The last property for F_2^1 is important because it shows that the modulus of the kernel *depends upon only one variable* as in the one-dimensional case. However no restriction appears for the phase of the kernel F_2^1. On the other hand, due to both Eqs. (12b), (13b), the modulus $|\widehat{K}_2^1|$ of the solution *depends also upon only one variable* $\xi_i x_i+x_j$. It follows that this is a very particular two-dimensional case because the modulus of the reconstructed potential depends in fact upon only one variable which is a linear combination of the two coordinates x_i (the same considerations about the phase hold as above). These properties will be useful later when we study the cases where the nonlinear part of Eq. (1) reduces to a purely cubic term.

5. The most simple degenerate case for the kernels F_j^i (a product of a function of s by a function of y) is very interesting because the solution of (3) can be written down in a closed form (it corresponds to the one soliton case in the one-coordinate case when the time is introduced):

$$F_j^i=g_j^i(s-x_j+x_i)\,h_j^i(y-x_i+x_j) \tag{14a}$$
$$D\widehat{K}_j^i=g_j^i(x_i)\,h_j^i(x_j)\,,$$
$$D\widehat{K}_i^i=g_i^i(x_j)\,h_j^i(x_j)\int_{x_i}^{\infty}g_j^i(w)\,h_i^j(w)\,dw\,,$$

$$D=1-\int_{x_1}^{\infty}g_2^1(w)\,h_1^2(w)\,dw\int_{x_2}^{\infty}g_1^2(w)\,h_2^1(w)\,dw\,. \tag{14b}$$

The main difference with the one-coordinate case is that g_j^i, and h_j^i do not need to be of a pure exponential type.

If we require now that $\widehat{K}_1^2=\eta\,\widehat{K}_2^{1*}$ (η real) we get:

$$F_2^1=g_1(s-x_2+x_1)g_2(y-x_1+x_2)\,, \tag{15a}$$
$$F_1^2=\eta\,[g_2(s-x_1+x_2)g_1(y-x_2+x_1)\,]^*,$$
$$D\widehat{K}_2^1=g_1(x_1)g_2(x_2)\,,$$
$$D\widehat{K}_i^i=\eta|g_j(x_j)|^2\int_{x_i}^{\infty}|g_i(w)|^2dw\,, \tag{15b}$$
$$D=1-\eta\int_{x_1}^{\infty}|g_1(w)|^2dw\int_{x_2}^{\infty}|g_2(w)|^2dw\,.$$

In Appendix A we prove for the particular solution [(15a) and (15b)] of Eq. (3) that if $(\partial/\partial x_i-\xi_i\partial/\partial x_j)\,\widehat{K}_i^i=0$, then $\xi_i\xi_j=1$ and $|g_i|$ are of pure exponential type. This alternative proof (in a particular case) of the more general property

(13a) and (13b) could be useful for the reader mainly interested in a simple solution like (15).

6. In Appendix A it is shown that if $F_1^2(u;\ v)=\eta\ [F_2^1(v;\ u)\ ]^*$, $F_2^1(u;\ v)=F_2^1(u+\xi v)$, then $\hat{K}_j^i$ depends upon one variable, $\hat{K}_j^i=\hat{K}_j^i(x_1+\xi x_2)$.

III. DERIVATION OF THE GENERALIZED NONLINEAR SCHRÖDINGER EQUATION IN TWO SPATIAL DIMENSIONS

In order to derive the evolution equations associated with Eq. (3) we adopt the same strategy as in the one-coordinate case.[6] First we introduce a parameter t in the kernel of Eq. (3), $\mathcal{F}(x_1,x_2;\ s;\ y;t)$, and differentiate with respect to t,

$$\mathcal{K}_t-\int\mathcal{F}_t\mathcal{K}=\widetilde{\mathcal{F}}_t+\int\mathcal{F}_t\mathcal{K}. \tag{16}$$

Secondly we want to compare the rhs of Eq. (16) with Eq. (3) itself. So we asume that $\mathcal{F}_t$ is linked either to $\mathcal{F}$ or to its derivatives with respect to the variables s,y,x_1,x_2. In this way the results of Sec. II.B will be applied. Thirdly, using straightforward but tedious calculations, we want, starting from Eq. (16), to deduce another integral equation proportional to Eq. (3).

1. We consider $F_j^i(s-x_j+x_i;\ y-x_i+x_j;\ t)$, $\widetilde{F}_j^i=F_j^i(x_i;\ y-x_i+x_j;\ t)$ in Eq. (3) and assume,

$$\left(\frac{i\partial}{\partial t}+\alpha_1\frac{\partial^2}{\partial s^2}+\alpha_2\frac{\partial^2}{\partial y^2}\right)F_2^1=0,$$
$$\left(-\frac{i\partial}{\partial t}+\alpha_1\frac{\partial^2}{\partial y^2}+\alpha_2\frac{\partial^2}{\partial s^2}\right)F_1^2=0, \tag{17}$$

where α_1 and α_2 are constants. Consequently for $\widetilde{\mathcal{F}}$ we get:

$$\left(\frac{i\partial}{\partial t}+\alpha_1O_{sx_1}^2+\alpha_2\frac{\partial^2}{\partial x_2^2}\right)\widetilde{\mathcal{F}}_2^1=0,$$
$$\left(-\frac{i\partial}{\partial t}+\alpha_1\frac{\partial^2}{\partial x_1^2}+\alpha_2O_{sx_2}^2\right)\widetilde{\mathcal{F}}_1^2=0,$$
$$\widetilde{F}_{2,y}^1=\widetilde{F}_{2,x_2}^1,\quad \widetilde{F}_{1,y}^2=\widetilde{F}_{1,x_1}^2 \tag{17a}$$

2. Using Eq. (17) in the rhs of Eq. (16) and some elementary algebra, we deduce an integral equation of the Eq. (10) type where

$$\mathcal{H}_{\rm III}=\begin{pmatrix}\frac{i\partial}{\partial t}+\alpha_2\frac{\partial^2}{\partial y^2} & 0\\ 0 & \frac{i\partial}{\partial t}-\alpha_1\frac{\partial^2}{\partial y^2}\end{pmatrix}\mathcal{K},$$

$$\mathcal{H}_{\rm III}^0=\begin{pmatrix}0 & \left(\frac{i\partial}{\partial t}+\alpha_2\frac{\partial^2}{\partial y^2}\right)\widetilde{F}_2^1\\ \left(\frac{i\partial}{\partial t}-\alpha_1\frac{\partial^2}{\partial y^2}\right)\widetilde{F}_1^2 & 0\end{pmatrix}$$

$$+\widetilde{\mathcal{F}}\begin{pmatrix}\alpha_2K_{1,y}^1|_{y=x_1} & \alpha_2K_{2,y}^1|_{y=x_1}\\ -\alpha_1K_{1,y}^2|_{y=x_2} & -\alpha_1K_{2,y}^2|_{y=x_2}\end{pmatrix}$$

$$+\begin{pmatrix}0 & F_{1,s}^2|_{s=x_1}\\ F_{2,s}^1|_{s=x_2} & 0\end{pmatrix}\begin{pmatrix}-\alpha_2\hat{K}_1^1 & -\alpha_2\hat{K}_2^1\\ \alpha_1\hat{K}_1^2 & \alpha_1\hat{K}_2^2\end{pmatrix}$$

3. Any linear combination of the $\mathcal{H}_i$ also has a structure of the type Eq. (10). We seek a combination such that the free term is proportional to $\widetilde{\mathcal{F}}$ and we get

$$\mathcal{H}_{\rm IV}=\mathcal{H}_{\rm III}+\mathcal{H}_{\rm II}\begin{pmatrix}-\alpha_2 & 0\\ 0 & \alpha_1\end{pmatrix}+\mathcal{H}_{\rm I}\begin{pmatrix}0 & \alpha_2\hat{K}_2^1\\ -\alpha_1\hat{K}_1^2 & 0\end{pmatrix},$$

$$\mathcal{H}_{\rm IV}^0=\widetilde{\mathcal{F}}\begin{pmatrix}2\alpha_2\hat{K}_{1,x_2}^1 & \alpha_2\hat{K}_{2,x_2}^1\\ -\alpha_1\hat{K}_{1,x_1}^2 & -2\alpha_1\hat{K}_{2,x_1}^2\end{pmatrix}.$$

Finally, we obtain

$$\mathcal{H}_{\rm IV}-\mathcal{K}\begin{pmatrix}2\alpha_2\hat{K}_{1,x_2}^1 & \alpha_2\hat{K}_{2,x_2}^1\\ -\alpha_1\hat{K}_{1,x_1}^2 & -2\alpha_1\hat{K}_{2,x_1}^2\end{pmatrix}=\begin{pmatrix}0&0\\0&0\end{pmatrix}. \tag{18}$$

Equation (18) gives us four scalar nonlinear partial differential equations (nlpde) for functions depending upon four variables x_1,x_2,y,t,

$$\left[\frac{i\partial}{\partial t}+\epsilon\alpha_j\left(\frac{\partial^2}{\partial y^2}-O_{dx_j}^2-2\hat{K}_{i,x_j}^i\right)\right]K_i^i$$
$$+\alpha_i[K_j^i\hat{K}_{i,x_j}^j-\hat{K}_i^jO_{s,x_j}K_j^i]=0,\quad i\neq j, \tag{18a}$$

$$\left(\epsilon\frac{i\partial}{\partial t}+\alpha_j\frac{\partial^2}{\partial x_j^2}+\alpha_iO_{s,x_i}^2\right)K_j^i+2\alpha_iK_j^i\hat{K}_{j,x_i}^j$$
$$+2\alpha_j\hat{K}_j^iK_{i,x_j}^i=0,\quad i\neq j, \tag{18b}$$

where $\epsilon=-1$ for $i=2$ and $\epsilon=+1$ for $i=1$.

Only $\hat{K}_j^i$, $i\neq j$ are linked to the potentials q_j^i of System (9). If we restrict Eq. (18b) to $y=x_i$ we get

$$\left(\epsilon i\frac{\partial}{\partial t}+\alpha_j\frac{\partial^2}{\partial x_j^2}+\alpha_i\frac{\partial^2}{\partial x_i^2}+2\alpha_i\hat{K}_{j,x_i}^j\right.$$
$$\left.+2\alpha_j\hat{K}_{i,x_j}^i\right)\hat{K}_j^i=0,\ i\neq j,$$
$$\hat{K}_{i,x_j}^i+\hat{K}_j^i\hat{K}_i^j=0. \tag{18c}$$

If, further, we link the two potentials $\hat{K}_2^1$ and $\hat{K}_1^2$ by assuming $\hat{K}_1^2=\eta\hat{K}_2^{1*}$, then both equations in (18c) are complex conjugate and finally we get the extension of the nonlinear Schrödinger equation in two spatial dimensions, written down in Eq. (1),

$$\left(\frac{i\partial}{\partial t}+\alpha_1\frac{\partial^2}{\partial x_1^2}+\alpha_2\frac{\partial^2}{\partial x_2^2}+2\alpha_1\hat{K}_{2,x_1}^2+2\alpha_2\hat{K}_{1,x_2}^1\right)\hat{K}_2^1=0,$$
$$\hat{K}_{i,x_j}^i+\eta|\hat{K}_2^1|^2=0. \tag{1'}$$

IV. SOLUTIONS OF THE GENERALIZED NONLINEAR SCHRÖDINGER EQUATION IN TWO SPATIAL DIMENSIONS

In principle we could consider any kernel $F_j^i(s-x_j+x_i;y-x_i+x_j;t)$ satisfying Eq. (17), the heat equation for imaginary time, and such that the boundary conditions (4a) and (4b) are satisfied. However, we focus our attention on:

(i) the study of Eq. (1). Thus $\hat{K}_1^2=\eta\,\hat{K}_2^{1*}$, $F_1^2(u;v;t)=\eta[F_2^1(v;u;t)]^*$, and our discussion is limited to $F_2^1(s-x_2+x_1;y-x_1+x_2;t)$ whereas $F_1^2(s-x_1+x_2;y-x_2+x_1;t)=\eta[F_2^1(y-x_2+x_1;s-x_1+x_2;t)]^*$.

(ii) the assumption that F_2^1 is a sum of a finite number of discrete terms (no continuum),

$$F_2^1=\sum_{i=1}^{N} a_i g_{1,i}(u_1=s-x_2+x_1;t)g_{2,i}(u_2=y-x_1+x_2;t), \tag{19}$$

$$F_1^2=\eta\sum_{i=1}^{N}[a_i g_{1,i}(y-x_2+x_1;t)g_{2,i}(s-x_1+x_2;t)]^*,$$

where the a_i are arbitrary constants and $g_{1,i}g_{2,i}$ is a solution of Eq. (17) for any i.

Due to the fact that the heat equation is of the first order in $\partial/\partial t$ and that the derivatives $\partial^2/\partial u_j^2$ apply only on $g_{j,i}(u_j,t)$, we get

$$\left(i\frac{\partial}{\partial t}+\alpha_j\frac{\partial^2}{\partial u_j^2}\right)g_{j,i}(u_j;t)=0. \tag{20}$$

Considering the general heat solution (with a time translation in order to have integrable Gaussian kernels) we get for the general kernel Eq. (19),

$$g_{j,i}(u_j)=(\mu_{j,i})^{-1/2}\times\int_{-\infty}^{+\infty}\exp[(u_j-u_j^1)^2]/\mu_{j,i}G_{j,i}(u_j^1)du_j^1, \tag{19a}$$

where $G_{j,i}(u_j^1)$ are arbitrary spectral functions such that F_2^1 leads to a correct formalism [Eqs. (4a) and (4b)] and $\mu_{j,i}=\eta_{j,i}-4i\alpha_j t$, $\mathrm{Re}\mu_{j,i}=\mathrm{Re}\eta_{j,i}<0$.

In the following we begin our study with the most degenerate case $N=1$ in Eq. (19) (corresponding to the one-soliton case in one dimension) where the solution is written down in closed form in Eq. (15b). We will have to consider only two $G_j(u_j^1)$, $j=1,2$ functions [we drop the subscript i in (19a)]. We want to illustrate some general features by some examples in both cases where the nonlinear part of (1) reduces or not to a cubic term. Introducing later other terms with $N>1$ (what is called multisoliton in one dimension), the solutions are not written down in closed form; however, we can still study these general features. For simplicity we disregard in our discussion the cases where the Fredholm determinant can vanish. However let us remark that in (15b), D is always different from zero for $\eta<0$. In the pure cubic case, we know (II B 3) that $|\hat{K}_2^1|$ depends upon only $x_1+\xi x_2$ (ξ real being a constant). In the x_1x_2 plane, along the asymptotic $x_1+\xi x_2=$ constant directions, $|\hat{K}_2^1|$ cannot be confined; and we want to verify this property with simple explicit examples.

$N=1$: First case: the nonlinear part of (1) does not reduce to a purely cubic term and we show that there exists an infinite number of solutions which are confined in the x_1x_2 plane.

Let us define $x_1=R\cos\theta$, $x_2=R\sin\theta$. We study $|\hat{K}_2^1|$ when $R\to\infty$. In the discussion we find two cases: Either the numerator $D|\hat{K}_2^1|\to 0$ and the Fredholm denominator D [Eq. (15b)] is bounded, or we have to investigate both the Fredholm numerator and denominator.

(i) Decreasing like a Gaussian at finite time

As a *first example* we take $G_j=\delta(u_j^1)$ in (19a) leading to $g_j=(\mu_j)^{-1/2}\exp(u_j^2/\mu_j)$ and we get the solution $\hat{K}_2^1=\phi$ written down in the Introduction [Eq. (2)]. In Eq. (2) the numerator goes to zero likes a Gaussian when $R\to\infty$ whereas the denominator D is bounded. We get $D<1+(|\eta|/2)[|\mathrm{Re}\mu_1\mathrm{Re}\mu_2|]^{-1/2}$. For $\eta<0$, $D>0$ whereas for $\eta>0$, D can be zero. For $\eta<2\pi^{-1}(|\mathrm{Re}\mu_1\mathrm{Re}\mu_2|)^{1/2}$, D is different than zero. We add $D\hat{K}_i^i$ in order to have all the quantities defined in Eq. (2),

$$D\hat{K}_i^i=\frac{\eta}{|\mu_j|}\frac{1}{(|\mathrm{Re}\mu_i|)^{1/2}}\times\exp\left[2x_j^2\frac{\mathrm{Re}\mu_j}{|\mu_j|^2}\right]\int_{\tilde{x}_i}^{\infty}dv_i\exp(-2v_i^2)$$

As a second *example* we take $G_j=\delta^1(u_j^1)$, leading to $g_j=u_j(\mu_j)^{-3/2}\exp(u_j^2/\mu_j)$ and get another solution of Eq. (1) confined in the x_1x_2 plane for finite time,

$$\hat{K}_2^1=\frac{\Pi_{j=1}^2(\mu_j)^{-3/2}x_j\exp(x_j^2/\mu_j)}{1-\eta\,\Pi_{j=1}^2|\mathrm{Re}\mu_j|^{-3/2}\int_{\tilde{x}_j}^{\infty}dv_j v_j^2\exp(-2v_j^2)}.$$

As a *third* case we consider a more general family of examples. We start from a linear combination of distributions for G_j,

$$G_j=\sum_q\rho_{j,q}\delta^{(2q)}(u_j^1)+\xi_{j,q}\delta^{(2q+1)}(u_j^1), \tag{21a}$$

where $\rho_{j,q}$ and $\xi_{j,q}$ are constant numbers. From the heat equation we get

$$g_j(u_j)=(\mu_j)^{-1/2}\exp(u_j^2/\mu_j)\sum_q\left(\rho_{j,q}\sum_{p=0}^{q}\frac{a_{p,2q}}{(\mu_j)^{p+q}}u_j^{2p}+\xi_{j,q}\sum_{p=0}^{q}\frac{a_{p,2q+1}}{(\mu_j)^{p+q+1}}u_j^{2p}\right) \tag{21b}$$

where the numbers $a_{p,2q}$ and $a_{p,2q+1}$ are easily computed. Substituting these expressions into Eq. (15b) we see that the confined properties of the solution in the x_1x_2 plane, at finite

time, are the same as in the previous examples. Here, we have a product of Gaussian functions by polynomials such that the asymptotic behavior in the x_1x_2 plane are dominated by the Gaussian terms.

(ii) Decreasing at least like an exponential (finite time)

As we shall see later, pure exponential g_j kernels do not lead to confined solutions. However as a *fourth* family of examples if we mix exponential type kernels with Gaussian type kernels, then the resulting solution $\hat{K}_2^1$ are still confined. However, for this property we have both to consider the numerator and the denominator. For instance, let us choose $g_1=\exp\eta_1(u_1+i\alpha_1\eta_1 t)$, $g_2=(\mu_2)^{-1/2}\exp(u_2^2/\mu_2)$, $\mathrm{Re}\eta_j<0$, $\mu_2=-4i\alpha_2 t+\eta_2$. Then we get

$$\hat{K}_2^1=(\mu_2)^{-1/2}\exp[i\phi+x_2^2/\mu_2]\{\exp(-\xi_1)$$

$$+[\eta\ \exp(\xi_1)/2\mathrm{Re}\eta_1\sqrt{|\mathrm{Re}\eta_2|}\,]$$

$$\times\int_{\tilde{x}_2}^{\infty}\exp(-2w^2\,dw)\Big\}^{-1}$$

$$\begin{cases}\xi_1=\mathrm{Re}\eta_1(x_1-2\alpha_1 t\,\mathrm{Im}\eta_1)\\ \phi=x_1\mathrm{Im}\eta_1+\alpha_1 t\,[(\mathrm{Re}\eta_1)^2-(\mathrm{Im}\eta_1)^2\,]\end{cases}, \tag{22}$$

where $\tilde{x}_2$ is the same as in Eq. (2).

The denominator is the Fredholm determinant multiplied by $\exp(-\xi_1)$. We recognize for x_2 fixed, the classical $[\cosh]^{-1}$ function, typical of the one-soliton solution in the one-coordinate case. Of course, instead of the pure Gaussian for g_2 we can choose any other function of the type (21b), the solution $\hat{K}_2^1$ being still confined in the x_1x_2 plane at finite time. We could also replace g_1 by an exponential multiplied by a polynomial as in the following.

(iii) Decreasing at least like powers

Let us consider for the g_j the product of an exponential by a polynomial of arbitrary order. The most simple cases are the zeroth, the first, or the second order. We can verify that the heat equation (20) has solutions (with, as before, $\mathrm{Re}\eta_j<0$):

$$g_j=\exp[\eta_j(u_j+i\alpha_j\eta_j t)], \tag{23a}$$

$$g_j=(u_j+2i\alpha_j\eta_j t)\exp[\eta_j(u_j+i\eta_j\alpha_j t)], \tag{23b}$$

$$g_j=(u_j^2+4i\alpha_j\eta_j u_j t+2i\alpha_j t-4\alpha_j^2\eta_j^2 t^2)\exp[\eta_j(u_j+i\eta_j\alpha_j t)], \tag{23c}$$

and so on for polynomials of higher order in u_j. We do not consider here both g_1 and g_2 given by Eq. (23a) [the resulting F_2^1 should lead to a pure cubic nonlinear part in Eq. (1)].

As a *first example* we take g_1 in (23a), g_2 in (23b) and get:

$$(\hat{K}_2^1)^{-1}=\Big(\exp[-(\xi+i\phi)]+\frac{\eta}{2\mathrm{Re}\eta_1}\exp(\xi-i\phi)$$

$$\times\int_0^{\infty}|v+x_2+2i\alpha_2\eta_2 t|^2\Big)\exp(2\mathrm{Re}\eta_2 v)dv]$$

$$\times(x_2+2i\alpha_2\eta_2 t)^{-1} \tag{24a}$$

$$\phi=\sum_{j=1}^{2}\alpha_j t\,\mathrm{Re}\eta_j^2+x_j\,\mathrm{Im}\eta_j,$$

$$\xi=\sum_{j=1}^{2}x_j\mathrm{Re}\eta_j-t\alpha_j\mathrm{Im}\eta_j^2.$$

Along the asymptotic directions $x_1\mathrm{Re}\eta_1+x_2\mathrm{Re}\eta_2=\mathrm{const}$, in the x_1x_2 plane, $|\hat{K}_2^1|$ decreases like a power R^{-1} whereas outside these directions, $|\hat{K}_2^1|$ decreases like an exponential.

As a *second example* we take both g_j in Eq. (23b) and get $(\hat{K}_2^1)^{-1}=[\exp[-(\xi+i\phi)]-\eta\ \exp(\xi-i\phi)$

$$\times\prod_{j=1}^{2}\int_0^{\infty}|v_j+x_j+2i\alpha_j\eta_j t|^2$$

$$\times\exp(2\mathrm{Re}\eta_j v_j)\,dv_j\Big]\Big[\prod_1^2(x_j+2i\alpha_j\eta_j t)\Big]^{-1}, \tag{24b}$$

where ϕ and ξ are the same as in Eq. (24a). We find that in the x_1x_2 plane, $|\hat{K}_2^1|$ decreases at least as R^{-2}. As a *third example* if g_1 is given by (23b) and g_2 by (23c), then $|\hat{K}_2^1|$ decreases at least as R^{-3}. Both g_j of the Eq. (23c) type lead to a decrease of at least R^{-4} and so on.

$N=1$: Second case: the nonlinear part of Eq. (1) is reduced to a purely cubic term and we show that the solutions are not confined in the x_1x_2 plane.

From the study of Sec. II B, we know that $|g_j|$ must be of the exponential type. As a first example we take the most simple case where both the modulus and the phase of g_j are exponential, or equivalently g_j are given by Eq. (23a). We get

$$(\hat{K}_2^1)^{-1}=\exp[-(\xi+i\phi)]-\frac{\exp(\xi-i\phi)}{4\mathrm{Re}\eta_1\mathrm{Re}\eta_2}, \tag{24c}$$

where ξ and ϕ are still given by Eq. (24a). This solution is the extension of the classical soliton solution in one-spatial dimension. Of course this solution is not confined along the direction $x_1\mathrm{Re}\eta_1+x_2\mathrm{Re}\eta_2=\mathrm{const}$. Further, $|\hat{K}_2^1|$ depends upon only one variable, $x_1\mathrm{Re}\eta_1+x_2\mathrm{Re}\eta_2$.

As a second example, we assume that only $|g_j|$ is exponential. From the heat (20) we have found the exponential type solution Eq. (23a) and another one (see Appendix B),

$$g_j(u_j)=(d_j-t)^{-1/2}\exp\Big\{(d_j-t)^{-1}\Big[c_j u_j+i\Big(-\frac{u_j^2}{4\alpha_j}+\alpha_j c_j^2\Big)\Big]\Big\}, \tag{25a}$$

where c_j and d_j are real and t is restricted so that $c_j(d_j-t)^{-1}<0$.

Substituting this expression in Eq. (15b) we get

$$(\hat{K}_2^1)^{-1}=\left[\prod_{j=1}^{2}(d_j-t)^{1/2}\right]$$

$$\times\left[\exp[-(\xi+i\phi)]-\frac{\eta\exp(\xi-i\phi)}{4|c_1c_2|}\right], \tag{25b}$$

$$\xi=\sum_{j=1}^{2}\frac{c_jx_j}{d_j-t},\quad \phi=\sum_{j=1}^{2}\frac{1}{d_j-t}\left(-\frac{x_j^2}{4\alpha_j}+\alpha_jc_j^2\right).$$

We verify of course the general result (12b) and (13b) that $|\hat{K}_2^1|$ depends upon only one variable ξ. This solution is pathological but we verify that along $\xi=$constant, it is not confined. We could also choose a mixed kernel where g_1 is purely exponential [Eq. (23a)] and g_2 of the Eq. (25a) type. We still get a nonconfined solution.

In conclusion, at this most degenerate case level we see that there exists an infinite number of confined solutions in the noncubic case whereas in the cubic case the few solutions that we get are not confined.

$N>1$: First case: there exists an infinite number of confined solutions when the nonlinear part of (1) is not a pure cubic term.

We consider for F_2^1 a finite sum of terms given by Eq. (19) and even if the solutions are too complicated to be written in closed form, we can study the confinement properties. We get for the solution of Eq. (3), the extension when $N>1$ of the Eq. (15b) solution for $N=1$:

$$\hat{K}_2^1=\sum_{m=1}^{N}g_{2,m}(x_2)\left[g_{1,m}(x_1)+\eta\sum_{l=1}^{N}C_{m,l}^1A_l\right],$$

$$A_l\left[1-\eta\sum_m C_{m,l}^1C_{m,l}^2\right]-\eta\sum_{l'\neq l}A_{l'}\sum_m C_{m,l}^2C_{m,l'}^1$$

$$=\sum_m g_{1,m}(x_1)\,C_{m,l}^2, \tag{26}$$

$$C_{m,l}^j=\int_{x_j}^{\infty}dv\,g_{j,m}(v;t)g_{j,l}^*(v;t)dv,$$

where for simplicity we take $a_m=1$ in Eq. (19).

We disregard from our discussion the zeros of the Fredholm determinants and we consider finite time. We assume for the kernels $g_{j,m}$ that they are of the type of Eqs. (21a) and (21b) (introducing a subscript m in $\mu_{j,m}$, $\rho_{j,q,m}$ and $\zeta_{j,q,m}$, $\mu_{j,m}=-4i\alpha_jt+\eta_{j,m}$, $\mathrm{Re}\eta_{j,m}<0$) decreasing like Gaussians (multiplied by polynomials). Firstly, we remark that for this family of kernels, the $|C_{m,l}^j|$ are bounded in the x_1x_2 plane.

From Eq. (21b) we see that the modulus of the integrands in $C_{m,l}^j$ are decreasing Gaussians multiplied by polynomials and so the integrals exist when $x_j\to\infty$. Secondly, when we solve the linear system [second line of Eq. (26)] we see that A_l can be written like $\Sigma_m g_{1,m}(x_1)E_{m,l}$ where these $E_{m,l}$ are bounded in the whole x_1x_2 plane. Thirdly, for $\hat{K}_2^1$ [first line of Eq. (26)] always appear either the factors $g_{2,m}(x_2)g_{1,m}(x_1)$ or $g_{2,m}(x_2)g_{1,l}(x_1)$ multiplied by bounded functions in the x_1x_2 plane and consequently $\hat{K}_2^1$ decreases like a Gaussian (multiplied by polynomials) when $R=(x_1^2+x_2^2)^{1/2}\to\infty$.

$N>1$: Second case: the solutions corresponding to a pure cubic term in Eq. (1) are not confined.

We recall that this property is a consequence of our general result of (II B). Namely $|\hat{K}_2^1|$ is a function of $x_1+\xi x_2$ and consequently in the asymptotic directions $x_1+\xi x_2=$const. of the x_1x_2 plane, $|\hat{K}_2^1|$ cannot be confined. We want to verify here this general property with some examples. We can choose in Eq. (19) a superposition of solutions $g_{j,l}(u_j;t)$ of type Eq. (23a) or (25a), restricted by the fact that as a function of $(u_1;u_2)$, $|F_2^1(u_1;u_2)|$ depends upon only $u_1+\xi u_2$. In this way we consider for instance two families of kernels,

$$F_2^1=\sum_{m=1}^{N}a_m\exp[\eta_m(u_1+\xi u_2)+it\eta_m^2(\alpha_1+\xi^2\alpha_2)]$$
$$\mathrm{Re}\eta_m<0 \tag{27}$$

$$F_2^1=\frac{1}{d-t}\exp\frac{i}{t-d}\left(\frac{u_1^2}{4\alpha_1}+\frac{u_2^2}{4\alpha_2}\right)\sum_{m=1}^{N}a_m$$

$$\times\exp\left[\frac{C_m}{d-t}[u_1+\xi u_2+iC_m(\alpha_1+\xi^2\alpha_2)]\right] \tag{28}$$

C_m,d are real, $C_m/(d-t)<0$.

In Eq. (27) both the phase and the modulus depend upon only $u_1+\xi u_2$. Following the result of Appendix A (quoted in II B 6), $\hat{K}_2^1$ depends upon only $x_1+\xi x_2$ and from the structures of both Eqs. (26) and (27), $\hat{K}_2^1$ is in fact a function of the variable exp[const.$(x_1+\xi x_2)$] which remains constant in the asymptotic directions $x_1+\xi x_2=$constant.

In Eq. (28), only $|F_2^1|$ depends upon $u_1+\xi u_2$. In Appendix B, for $N=2$, we explicitly show that $|\hat{K}_2^1|$ depends upon only one variable exp[const.$(x_1+\xi x_2)$], and consequently in the x_1x_2 plane $|\hat{K}_2^1|$ cannot be confined.

V. CONCLUSION

In this paper, for two different cases, we have studied the confinement properties of the solutions of the nonlinear Schrödinger equation, in a two-dimensional space (x_1,x_2):

(i) If the nonlinear part is reduced to a purely cubic term (as in the one-dimensional case), we show that the modulus of the solution depends in fact upon one coordinate $x_1+\xi x_2$. Consequently the solutions cannot be confined in the x_1x_2 plane.

(ii) If the nonlinear part is not reduced to the usual cubic term, but is like the extensions previously found by Ablowitz, Haberman,[1] and Morris,[4] then there exists an infinite number of confined solutions at any finite time.

Although we have focused here our attention on the existence and confinement properties of the solutions, there

remain of course other problems: a possible extension in a three-dimensional space, the existence (or not) of conservation laws... .

There exist classical nonlinear evolution equations for which we know that the extension to more than one spatial dimension should lead to difficulties concerning the existence of the solutions. The nonlinear Schrödinger example may provide a possible escape from these difficulties. The way being not only in the trivial changes of the linear part (where derivatives with respect to one coordinate must be replaced by the corresponding ones with many coordinates) but also in the modification of the nonlinear part. The fact that for this example, the same extension has been obtained by three different methods indicates that this extension certainly has a deep meaning. Perhaps an approach[3] like the "prolongation structure" is convenient to understand the modifications to be introduced going in higher dimensions.

In the inversionlike formalism these extensions are very natural because they introduce into the resulting nonlinear evolution equations, the solutions of the IE which are not directly linked to the potentials. For instance in a 2×2 IE, the $\hat{K}_i^i$ functions are introduced in supplement to the $\hat{K}_j^i (i\neq j)$ which are the potentials of the associated partial differential systems. These inversionlike integral equations appear as a powerful tool for the study of higher dimensional nlpde and it remains now to study the extensions of the other classical nlpde.

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APPENDIX A

1. Firstly we investigate the properties for $\hat{K}_j^i$, due to the assumption

$$F_1^2(u,v)=\eta\,[F_2^1(v,u)\,]^*,\quad \eta \text{ real.} \tag{A1}$$

We iterate Eq. (11) and get:

$$\hat{K}_j^i=F_j^i(x_i,x_j)+\sum_{n=1}^{\infty}\int_{x_j}dr_1\cdots\int_{x_j}dr_n\int_{x_i}dv_1\cdots\int_{x_i}dv_n$$

$$\times F_j^i(r_1,x_j)\,F_i^j(v_1,r_1)\left[\prod_2^n F_j^i(r_i,v_{i-1})F_i^j(v_i,r_i)\right]$$

$$\times F_j^i(x_i,v_n)\,, \tag{A2}$$

$$\hat{K}_i^i=\sum_{n=0}^{\infty}\int_{x_i}dv_0\cdots\int_{x_i}dv_n\int_{x_j}dr_1\cdots\int_{x_j}dr_n F_j^i(v_0,x_j)$$

$$\times\left[\prod_1^n F_i^j(r_i,v_{i-1})\,F_j^i(v_i,r_i)\right]F_i^j(x_j,v_n)\,, \tag{A3}$$

where in (A3) $\prod_1^n$ reduces to 1 for $n=0$. Taking into account (A1) we get:

$$\eta^{-1}\hat{K}_1^{2*}=F_2^1(x_1,x_2)$$

$$+\sum_{n=1}^{\infty}\int_{x_1}dr_1\cdots\int_{x_1}dr_n\int_{x_2}dv_1\cdots\int_{x_2}dv_n F_2^1(x_1,r_1)\,F_1^2(r_1,v_1)$$

$$\times\left[\prod_2^n F_2^1(v_{i-1},r_i)\,F_1^2(r_i,v_i)\right]F_2^1(v_n,x_2) \tag{A4}$$

$$\hat{K}_i^{i*}=\sum_{n=0}^{\infty}\int_{x_i}dv_0\cdots\int_{x_i}dv_n\int_{x_j}dr_1\cdots\int_{x_j}dr_n F_i^j(x_j,r_0)$$

$$\times\left[\prod_1^n F_j^i(v_{i-1},r_i)\,F_i^j(r_i,v_i)\right]F_j^i(v_n,x_j)\,. \tag{A5}$$

If in (A4) we exchange $r_i\Leftrightarrow v_{n-i+1}$, then the rhs of (A4) is just $\hat{K}_2^1$. If in (A5) we exchange $r_i\Leftrightarrow r_{n-i+1}$, $v_i\Leftrightarrow v_{n-i}$, then the rhs of (A5) is just $\hat{K}_i^i$.

So $\hat{K}_i^i$ is real and consequently if we define $|F_2^1(u,v)|=f(u,v)$, (A3) can be rewritten

$$\hat{K}_i^i=\sum_n\eta^n\int_{x_i}dv_0\cdots\int_{x_i}dv_n\int_{x_j}dr_1\cdots\int_{x_j}dr_n f(v_0,x_j)$$

$$\times\left[\prod_1^n f(v_{i-1},r_i)f(v_i,r_i)\right]f(v_n,x_j)\,. \tag{A6}$$

2. In addition to (A1) we assume

$$\left(\frac{\partial}{\partial x_1}-\zeta_1\frac{\partial}{\partial x_2}\right)\hat{K}_1^1=0. \tag{A7}$$

From

$$\left[\frac{\partial}{\partial\eta^n}\left(\frac{\partial}{\partial x_1}-\zeta_1\frac{\partial}{\partial x_2}\right)\hat{K}_1^1\right]_{\eta=0}=0$$

we see that (A7) must be true at each order in η. At the first order, we must have

$$\left(\frac{\partial}{\partial x_1}-\zeta_1\frac{\partial}{\partial x_2}\right)\int_{x_1}^{\infty}f^2(v_0,x_2)dv_0=0\,,$$

$$-f^2(x_1,x_2)=\zeta_1\int_{x_1}^{\infty}dv_0\frac{\partial}{\partial x_2}f^2(v_0,x_2)\,. \tag{A8}$$

If we differentiate both sides of (A8) with respect to x_1 we get

$$\left(\frac{\partial}{\partial x_1}-\zeta_1\frac{\partial}{\partial x_2}\right)f(x_1,x_2)=0, f(u,v)=f(\zeta_1 u+v). \tag{A9}$$

Taking into account (A9) into (A6), $\hat{K}_i^i$ can be rewritten

$$\hat{K}_1^1=\sum\eta^n\int_{x_1}dv_0\cdots\int_{x_1}dv_n\int_{x_2}dr_1\cdots\int_{x_2}dr_n f(\zeta_1 v_0+x_2)$$

$$\times\left(\prod_1^n f(\zeta_1 v_{i-1}+r_i)f(\zeta_1 v_i+r_i)\right)f(\zeta_1 v_n+x_2)\,, \tag{A10}$$

$$\hat{K}_2^2=\sum\eta^n\int_{x_2}dv_0\cdots\int_{x_2}dv_n\int_{x_1}dr_1\cdots\int_{x_1}dr_n f(v_0+\zeta_1 x_1)$$

$$\times\left(\prod_1^n f(\zeta_1 r_i+v_{i-1})f(\zeta_1 r_i+v_i)\right)f(v_n+\zeta_1 x_1)\ . \tag{A11}$$

If in (A10) we define $\zeta_1 v_i+x_2=W_i$, $r_i+\zeta_1 x_1=R_i$, in (A11) $\zeta_1 x_1+v_n=W_i$, $\zeta_1 r_i+x_2=R_i$ and in both cases $x=x_2+x_1\zeta_1$ we get

$$\zeta_1\hat{K}_1^1=\hat{K}_2^2$$

$$=\sum\eta^n\zeta_1\int_x dw_0\cdots dw_n\,dR_1\cdots\int_x dR_n f(w_0)f(w_n)$$

$$\times\prod_1^n f(w_{i-1}+R_i-x)f(w_i+R_i-x). \tag{A12}$$

From (A12) it is clear that both $\hat{K}_1^1$ and $\hat{K}_2^2$ are functions of one variable $x_2+x_1\zeta_1$. Further $(\partial/\partial x_2-\zeta_2\partial/\partial x_1)\hat{K}_2^2=0$ with $\zeta_2\zeta_1=1$. As a consequence, if f in (A9) is purely degenerate, it must be the product of two purely exponential functions.

3. We shall get the same property as in 2 for the particular solution written down in (15a) and (15b). We require

$$\left(\frac{\partial}{\partial x_i}-\zeta_i\frac{\partial}{\partial x_j}\right)\hat{K}_i^i=0 \tag{A13}$$

and define in Eq. (15) $|g_1(x_1)|^2=g(x_1)$, $|g_2(x_2)|^2=h(x_2)$. We get from Eq. (15)

$$gC_1+C_2\int g+C_3\left(\int g\right)^2=0, \tag{A14a}$$

$$gC_1+C_4\,g_{x_1}+C_5\left[g_{x_1}\int g+g^2\right]=0, \tag{A14b}$$

$$C_1=h,\ C_2=\zeta_1 h_{x_2},\ C_3=-\zeta_1 h\left[h_{x_2}\int h+h^2\right], \tag{A14c}$$

$$C_4=\zeta_2\int h,\quad C_5=-\eta\zeta_2\left(\int h\right)^2,$$

where $C_1\not\equiv 0$, $C_2\not\equiv 0$, $C_4\not\equiv 0$, $C_5\not\equiv 0$, C_3 can be zero.

We take the derivation of (A14a) with respect to x_1, get $C_1 g_{x_1}=gC_2+2C_3 g\int g$ and substitute in (A14b),

$$C_1^2+\left[C_4+C_5\int g\right]\left[C_2+2C_3\int g\right]+gC_1C_5=0. \tag{A15}$$

We multiply (A14a) by C_5 and subtract it from (A15),

$$[C_1^2+C_2C_4\ ]+2C_3C_4\int g+C_3C_5\left(\int g\right)^2=0. \tag{A16}$$

Thus $\int_{x_1}^\infty g(u)du$ is the solution of a second order algebraic equation with coefficients independent of x_1. This is impossible unless all the coefficients are zero, $C_1^2+C_2C_4=0$ or $h^2+\zeta_1\zeta_2 h_{x_2}\int h=0$ and $C_3=0$. Or

$$h^2+h_{x_2}\int_{x_2}^\infty h(u)du=0. \tag{A17}$$

Finally $\zeta_1\zeta_2=+1$ and the h_1 solution of (A17) is necessarily a pure exponential type function.

Let us remark that (A14) can also be written

$$hD_1+h_{x_2}D_4+D_5\left(h_{x_2}\int h+h^2\right)=0, \tag{A14a}$$

$$hD_1+D_2\int h+D_3\left(\int h\right)^2=0, \tag{A14b}$$

$$D_1=g\quad D_2=\zeta_2 g_{x_1},\quad D_3=-\zeta_2\eta\left[g_{x_1}\int g+g^2\right],$$

$$D_4=\zeta_1\int g,\quad D_5=-\eta\zeta_2(h)^2.$$

D_1, D_2, D_4, and D_5 are not equal to zero whereas D_3 can vanish. Doing the same analysis as before, we get $\zeta_1\zeta_2=1$ and

$$g^2+g_{x_1}\int g=0, \tag{A18}$$

which says that g also is a pure exponential function.

4. We assume

$$F_1^2(u;v)=\eta(F_2^1(v;u))^*,\quad F_2^1(u;v)=F_2^1(u+\xi v) \tag{A19}$$

and want to show $\hat{K}_j^i=\hat{K}_j^i(x_1+\xi x_2)$.

With (A19), Eq. (3) can be rewritten

$$\mathcal{K}(x_1,x_2;y)=\tilde{\mathcal{F}}(x_1,x_2;y)+\int_{-\infty}^{+\infty}\mathcal{T}(x_1,x_2;s;y)\mathcal{K}(x_1,x_2;s)ds,$$

$$\tilde{\mathcal{F}}=\begin{pmatrix}0 & F_2^1(x_1+\xi(y-x_1+x_2))\\ \eta F_2^{1*}(y-x_2+x_1+\xi x_2) & 0\end{pmatrix},$$

$$\mathcal{T}\begin{pmatrix}0 & F_2^1(s-x_2+x_1+\xi(y-x_1+x_2))\theta(s-x_1)\\ \eta(F_2^1(y-x_2+x_1+\xi(s-x_1+x_2)^*\theta(s-x_1) & 0\end{pmatrix}.$$

We define $K_j^i(x_1,x_2;y=x_i+z)=G_j^i(z)$, $x=x_1+\xi x_2$ and from (A21) we get

$$\begin{pmatrix}G_1^1(z) & G_2^1(z)\\ G_1^2(z) & G_2^2(z)\end{pmatrix}=\begin{pmatrix}0 & F_2^1(x+\xi z)\\ \eta(F_2^1(x+z))^* & 0\end{pmatrix}+\int_0^\infty du\begin{pmatrix}0 & F_2^1(\xi z+x+u)\\ \eta F_2^{1*}(z+x+\xi u) & 0\end{pmatrix}\times\begin{pmatrix}G_1^1(u) & G_2^1(u)\\ G_1^2(u) & G_2^2(u)\end{pmatrix}. \tag{A21}$$

From (A21) it is clear that $G_j^i(z)$ depends upon two variables x and z. Furthermore $\hat{K}_j^i = G_j^i(z=0)$ and it follows that $\hat{K}_j^i$ depends only upon x.

APPENDIX B

1. We want to find the general solution of the heat equation (for imaginary time),

$$\left(i\frac{\partial}{\partial t}+\alpha\frac{\partial^2}{\partial u^2}\right)F(u,t)=0 \quad \alpha \text{ real}, \tag{B1}$$

when $|F|$ is a purely exponential function of u. We define $F=|F(u,t)|\exp i\phi(u,t)$, $|F|=g(t)\exp(u\eta(t))$ and we get from (B1)

$$\frac{g_t}{\alpha g}+\frac{u}{\alpha}\eta_t+\phi_{uu}+2\phi_u\eta=0, \tag{B2}$$

$$\frac{\phi_t}{\alpha}=\eta^2-(\phi_u)^2. \tag{B3}$$

From (B2) we get

$$\phi=\frac{D_0(t)}{4\eta^2}\exp(-2\eta u)-\frac{\eta_t}{4\alpha\eta}u^2$$

$$+\frac{u}{\alpha}\left(\frac{\eta_t}{4\eta^2}-\frac{(\log g)_t}{2\eta}\right)+\frac{D_1(t)}{\alpha}, \tag{B4}$$

where D_0 and D_1 are arbitrary functions. However due to (B3) we have $D_0\equiv 0$. We get two cases following $\eta_t\equiv 0$ or $\eta_t\not\equiv 0$.

(i) $\eta_t\not\equiv 0$, we get

$$F=\exp d(u+id\alpha t), \quad d=\text{complex constant}. \tag{B5}$$

(ii) $\eta_t\not\equiv 0$. From (B3)–(B4) we get

$$\frac{\partial^2}{\partial t^2}\log\eta=\left(\frac{\partial}{\partial t}\log\eta\right)^2 \quad \text{or} \quad \eta=\frac{c}{(d-t)},$$

where c and d are arbitrary constants. Further we get $\frac{1}{2}(\log g)_{tt}-(\log g)_t(\log\eta)_t+\frac{1}{4}[(\log\eta)_t]^2=0$ or $g=(d_0-t)^{-1/2}$ and finally $D_1=\alpha^2c^2/(d-t)$,

$$F=(d-t)^{-1/2}\exp\frac{1}{d-t}\left[cu+i\left(-\frac{u^2}{4\alpha}+\alpha c^2\right)\right]. \tag{B6}$$

2. We consider the solutions Eq. (26) corresponding to the kernels Eq. (28) for $N=2$. t is fixed, we study the x_1,x_2 dependence of $\hat{K}_2^1$ and show that $|\hat{K}_2^1|$ depends only upon a function of $\exp\gamma_m(x_1+\xi x_2)$ where the γ_m are real. In Eq. (26) we have

$$g_{1,m}(u_1)=\frac{a_m}{\sqrt{d-t}}\exp\frac{1}{d-t}$$

$$\times\left(C_m(u_1+iC_m\alpha_1)-i\frac{u_1^2}{4\alpha_1}\right), \tag{B7}$$

$$g_{2,m}(u_2)=\frac{1}{d-t}\exp\frac{1}{d-t}$$

$$\times\left(C_m\xi(u_2+iC_m\xi\alpha_2)-i\frac{u_2^2}{4\alpha_2}\right).$$

Let us call H the space of functions constant. $\exp\gamma_m(x_1+\xi x_2)$; if $h_1\in H$, $h_2\in H$, then $h_1h_2\in H$. From Eqs. (26) and (B7) we get the rules (let us call $\tilde{H}$ the space of functions Σ const.$_i h_i$ with $h_i\in H$):

$$\begin{aligned}
&\text{(i) } C_{ml}^1C_{ml}^2\in H,\ C_{l,m}^1C_{m,l}^2\in H,\\
&\text{(ii) } C_{ml}^iC_{lm}^jC_{ll}^jC_{mm}^j\in H, \quad i\neq j,\\
&\text{(iii) } |g_{1m}(x_1)g_{2m}(x_2)|\in H,\\
&\text{(iv) } |g_{2m}(x_2)g_{1p}(x_1)|C_{mq}^1C_{pq}^2\in H, \quad m\neq p.
\end{aligned} \tag{B8}$$

$\hat{K}_2^1$ in Eq. (26) can be written N/D where D is the Fredhold determinant,

$$D=1-\eta\sum_{i=1}^{2}C_{i1}^1C_{i1}^2+C_{i2}^2C_{i2}^1+\eta^2\sum_{k=1}^{2}C_{k1}^1C_{l2}^2\sum_{i=1}^{2}C_{i2}^2C_{j1}^2, \quad i\neq j. \quad l\neq k. \tag{B9}$$

From (i) and (ii) we get $D\in\tilde{H}$ and from (iii) $D|\Sigma g_{2m}(x_2)g_{1m}(x_1)|\in\tilde{H}$. N is

$$N=D\hat{K}_2^1=D\sum_m g_{2m}(x_2)g_{1m}(x_1)$$

$$+\eta\sum_m\sum_p g_{2m}(x_2)g_{1p}(x_1)B_{m,p}, \tag{B10}$$

where the $B_{m,p}$ can be constructed from the $C_{m,l}^j$. Due to the fact that the u_j dependence of the phase in $g_{j,m}(u_j)$ [given by (B7)] is independent of m, the dependence in x_1x_2 of the phase in both the two terms at the rhs of (B10) is the same and can be factorized out. Now

$$B_{m,m}=C_{m,1}^1C_{m,1}^2\left[1-\eta\sum_i C_{i2}^1C_{i2}^2\right]$$

$$+C_{m,2}^1C_{m,2}^2\left[1-\eta\sum_i C_{i1}^1C_{i2}^2\right]$$

$$+\eta\Big[2C_{m,1}^1C_{m,1}^2C_{m,2}^2C_{m,2}^1$$

$$+\sum_{i=1}^{2}C_{i1}^1C_{j2}^1C_{j1}^2C_{i2}^2\Big], \quad i\neq j,$$

and applying rules (i) and (ii) we get that $B_{mm}\in\tilde{H}$. For $m\neq p$ we get for the second term on the rhs of (B10)

$$\eta g_{2m}(x_2)\, g_{1p}(x_1)\left\{C^1_{m,1}C^2_{p1}\left[1-\eta\sum_i C^1_{i2}C^2_{i2}\right]\right.$$

$$+C^1_{m2}C^2_{p2}(1-\eta\sum_i C^1_{i1}C^2_{i2})+C^2_{p2}C^1_{m2}C^1_{m1}C^2_{m1}$$

$$+C^1_{m1}C^2_{p1}C^1_{p2}C^2_{p2}+C^2_{p1}C^1_{m1}C^1_{m2}C^2_{m2}$$

$$\left.+C^1_{m,2}C^2_{p2}C^2_{p1}C^1_{p1}\right\}$$

such that applying rules (i), (ii), (iv) we see that the modulus belongs to H. Finally $|D\hat{K}^1_2|\in\tilde{H}$.

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Independence of the free energy for one-dimensional systems of fermions

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In this paper we prove the independence of the free energy of a one-dimensional system of fermions in a box from the boundary conditions by using the Wiener integral techniques.

INTRODUCTION

It is known that the methods of functional integration have been introduced in statistical mechanics by Ginibre[1] to study the correlation functions and the pressure of quantum systems of particles. By making use of these methods Novikov[2] has proved the independence of the free energy from the boundary conditions for systems of particles obeying Maxwell–Boltzmann or Bose–Einstein statistics, when the interaction is either hard core either positive and the boundary conditions are of the type

$$\left.\frac{\partial u}{\partial n}\right|_{\partial\Lambda} = ku, \quad 0 \leqslant k \leqslant +\infty,$$

where $\partial/\partial n$ denotes the inward normal derivative.[3] Similar results have been obtained by Gallavotti and Lupini.[4] In Ref. 4 a diffusion process with absorbing boundary was used to treat the cases $0 < k < +\infty$ (see also Ref. 7). The case $k < 0$ corresponds, as is shown in Ref. 8, to a process with creation of particles on the boundary.

The independence of the free energy from conditions for a one-dimensional system of interacting fermions is proven in our work for $-\infty < k \leqslant +\infty$, without the assumption of hard core. In this case the effect of boundary conditions is weakened in the process because of the condition of the particles of not touching one another. An interesting problem is to examine the dependence of the free energy for a one-dimensional system of interacting bosons with $k < 0$ (see Ref. 5).

Another approach to the problem of the independence of the free energy from the boundary conditions is due to Robinson.[6] He studies the Hamiltonians for different boundary conditions by looking at the corresponding quadratic forms; however it does not seem that in this way it is possible to treat the general interactions to which the method of functional integration applies.

1. DEFINITIONS AND CONDITIONS

We consider a system of N particles obeying Fermi–Dirac statistics, enclosed in a one-dimensional box Λ. The Hamiltonian of the system is formally defined by

$$H_n = -\tfrac{1}{2}\sum_{i=1}^{n}\frac{d^2}{dx_i^2} + \sum_{i<j}\Phi(|x_i - x_j|)$$

$$= -\tfrac{1}{2}\sum_{i=1}^{n}\frac{d^2}{dx_i^2} + U_N(x_1,\ldots x_N), \tag{1.1}$$

i.e., we assume that the particles interact through a pair potential depending only on the distance. We require that the function Φ only satisfy the following conditions:

(i) $\Phi(r)$ is continuous for every $r > 0$,

(ii) $\Phi(r) > -C$, $\forall\, r$, where C is some positive constant,

(iii) $|\Phi(r)| < (r^{1+\epsilon})^{-1}$ for $r > a'$, where ϵ and a' are some positive constant,

(iv) Φ is stable, that is $\sum_{1\leqslant i<j\leqslant N}\Phi(|x_i - x_j|) \geqslant -BN$, $\forall$ N, $\forall$ $(x_1,\ldots x_n)$, where $B > 0$ is a constant.

The proof also applies if the potential is hard core, i.e., for some $a > 0$, $\Phi(r) = +\infty$, for $0 \leqslant r \leqslant a$. In this case, however, the proof is easier. We will define the operator H_N through the Wiener integral technique. We first define an operator T_n in $L^2(\Lambda^N)$ which is a self-adjoint extension of the operator T'_N whose domain is $C_k^2(\Lambda^N)$, i.e., the space of the functions $\psi(x)$ twice differentiable with continuity until the boundary $\partial\Lambda^N$

$$k\psi((x^N)) - \frac{\partial\psi}{\partial n}((x^N)) = 0, \quad -\infty < k \leqslant +\infty,$$
$$(x^N) \in \partial\Lambda^N \setminus \Gamma^N, \tag{1.2}$$

where Γ^N is the set of the "corners" of the boundary $\partial\Lambda^N$ that is the set of the intersections of more than one $(N-1)$-dimensional face of $\partial\Lambda^N$, and $\partial/\partial n$ denotes the inward normal derivative. If $k = +\infty$, the condition (1.2) means $\psi((x^N)) = 0$.

The operator T_N^k can be defined as the product

$$\underbrace{T_1^k \otimes \cdots \otimes T_1^k}_{N \text{ times}}$$

where each of the operators T_1^k is defined through the Wie-

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ner integral technique (see Appendix A and for details see Refs. 7 and 8). In the case $k<0$ the operator $e^{-tT_N^k}$ can therefore be written in the following,

$$[e^{-tT_N^k}\psi](x^N) = E^k_{(x^N)}\Big[\sum_{\substack{i_1\in J_t^1\\ \dots\\ i_N\in J_t^N}} \psi(\omega_{i_1}(t),\dots,\omega_{i_N}(t))\Big], \tag{1.3}$$

where $E^k_{(x^N)}$ denotes the expectation with respect to N independent diffusion processes with creation on the boundary with initial points $x_1,x_2,\dots,x_N$, respectively, and J_t^l is the set of the indices of the particles of the l th process which are present at the instant t.

In the case of Fermi–Dirac statistics the domain of the operator $e^{-\beta H_N}$ is restricted to the antisymmetrical functions on which the scalar product

$$(\psi,\varphi)=\frac{1}{N!}\int_{\Lambda^N}\bar\psi(x)\varphi(x)dx \quad \text{is defined.}$$

In this case we can note the following. It follows from the well known properties of the Brownian motion that if two particles belonging to different processes hit each other, the successive part of their paths can be exchanged without changing the probability of the process.

Since the function $\psi(x)$ in (1.3) is antisymmetrical, the exchanged paths give the integral in (1.3) contributions equal in modulus with the sign of the corresponding permutation; it is easy to see that after all the cancellations, only those indices $i_1,\dots,i_N$ must be considered in the sum of (1.3) whose paths have never touched each other (where the path $\bar\omega_{i_l}$ corresponding to the index i_l is the path that starts from the ancestor of the particle i_l at the instant $t=0$ and follows the genealogical line that leads to the particle i_l).

If we define the function

$$\alpha(\bar\omega^N)=\alpha(\bar\omega_1,\dots,\bar\omega_N)$$

$$=\begin{cases}1 & \text{if } \forall\ s\in[0,t],\ \forall\ i,j\leqslant N,\quad i,j\geqslant 0,\ \bar\omega_i(s)\neq\bar\omega_j(s),\\ 0 & \text{otherwise,}\end{cases}$$

the expression (1.3) with antisymmetrical ψ can be written in the form

$$[e^{-tT_N^k}\psi](x^N) = E^k_{(x^N)}\Big[\sum_{\substack{i_1\in J_t^1\\ \dots\\ i_N\in J_t^N}} \psi(\bar\omega_{i_1}(t),\dots,\bar\omega_{i_N}(t))\alpha(\bar\omega_{i_1},\dots,\bar\omega_{i_N})\Big]. \tag{1.3'}$$

We can now define the operator $e^{-\beta(T_N^k+U_N)}$ through the usual construction which is motivated by Trotter's formula (see Ref. 3) in the following way,

$$[e^{-\beta(T_N^k+U_N)}\psi](x^N) = \int dP^{(k)}_{(x^N)(\bar\omega^N)}\sum_{i_1\cdots i_N}[\psi(\bar\omega_{i_1}(\beta),\dots,\bar\omega_{i_N}(\beta))]$$

$$\times\alpha(\bar\omega_{i_1},\dots,\bar\omega_{i_N})\exp\Big[-\int_0^\beta U_N(\bar\omega^N(s))ds\Big] \tag{1.4}$$

where $\bar\omega^N=(\bar\omega_{i1},\dots,\bar\omega_{i_N})$ and the integral is computed with respect to the measure $dP^k_{x^N}$ which is the measure associated with the process previously defined, with starting points $(x^N=x_1,\dots,x_N)$. Take as $\psi((x^N))$ the indicator of a set of Λ^N,

$$\psi((x^N))=\prod_{i=1}^N x_{A_i}(x_i), \text{ where } A_i\subset\Lambda. \tag{1.5}$$

From (1.4) it follows that

$$[e^{-\beta(T_N^k+U_N)}\psi](x^N) \leqslant\prod_{i=1}^N[E^k_{x_i}(N^t_i(A_i))]e^{\beta[N(N-1)C]/2}, \tag{1.6}$$

where $E^k_{x_i}(N^t_i(A_i))$ is the expectation value of the number of the descendants of ith particle that at the instant t lies in the set A; since $E^k_{x_i}(N^t_i(A_i))=0$ if the Lebesque measure of the set A_i is equal to zero, by the Radon Nikodim theorem the integral in (1.4) can be written in the form

$$\int K((x)^N,(y)^N)\psi((y)^N)dy^N, \tag{1.7}$$

where $K((x)^N,(y)^N)$ is a suitable density function with respect to the Lebesque measure. By virtue of the uniqueness of the conditional probability, up to null measure sets, we get

$$K((x)^N,(y)^N) = \int P^{(k)}_{(x^N),(y^N)}(d\omega)\alpha(\bar\omega^N)\exp[-U(\bar\omega)]$$

where $P^{(k)}_{(x^N),(y^N)}$ is the probability measure of our process with the condition that a descendant of the particle placed in x_l at the instant $t=0$ occurs in y_l at the instant $t=\beta$, $l=1,2,\dots,N$ and $\bar\omega^N=(\bar\omega_1,\dots,\bar\omega_N)$ are the corresponding lines of descendence. So we can conclude

$$\mathrm{Tr}e^{-\beta H_N^k} = \frac{1}{N!}\int_{\Lambda^N}K((x^N),(x^N))\,d(x)^N$$
$$=\frac{1}{N!}\int P^k_{(x^N),(x^N)}(d\omega)\alpha(\bar\omega^N)\exp[-U(\bar\omega)]dx^N.$$

2. INDEPENDENCE FROM THE BOUNDARY CONDITIONS

The free energy of the system corresponding to the boundary conditions

$$\left.\frac{\partial\psi}{\partial n}\right|_{\partial\Lambda}=k\psi$$

is defined in this way,

$$f^k(\rho,\beta)=\lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} -\frac{1}{\beta}\frac{\log Z^k(N,\Lambda,\beta)}{N}, \tag{2.1}$$

where $Z(N,\Lambda,\beta)$ is the partition function of the canonical ensemble

$$Z^k=\mathrm{Tr}e^{-\beta H^k_{N,\Lambda}} \tag{2.2}$$

[the minus sign shows that the operator in (2.2) is restricted to skew functions].

Now we want to prove the following theorem:

Theorem 1: If the limit (2.1) with $k=\infty$ exists and the potential function satisfies conditions (i)–(iv), then for every k, $-\infty<k<+\infty$, the limit (2.1) exists and

$$f^k(\rho,\beta)=f^{+\infty}(\rho,\beta), \tag{2.3}$$

that is the limit is independent on and is equal to the null boundary conditions limit.

Before the proof we want to exhibit a bound for Tr $e^{-\beta T^k_{1,\Lambda}}$. It is true that

$$\mathrm{Tr}e^{-\beta T^k_{1,\Lambda}}=\sum_i e^{-\beta\lambda_i}$$

where λ_i are the eigenvalues of $T^k_{1,\Lambda}$. It is well known that for $k<0$ there are at most two negative eigenvalues which tend to $-k^2$ whereas the positive ones satisfy the chain of inequalities

$$\left(\frac{\pi}{|\Lambda|}\right)^2<\left(\frac{2\pi}{|\Lambda|}\right)^2<\lambda_3<\cdots.$$

Finally

$$\mathrm{Tr}e^{-\beta T^k_{1,\Lambda}}\leqslant 2e^{2k^2}+e+\sum_{n=1}^{\infty}\exp\left[-\beta\left(\frac{n\pi}{|\Lambda|}\right)^2\right]$$

$$\leqslant 2e^{2k^2}+e+\frac{|\Lambda|}{\pi}$$

$$\times\int_0^{\infty}e^{-\beta x^2}dx\leqslant|\Lambda|,$$

where Q is some constant (see Ref. 5).[9]

We go on now with the proof of the theorem. First, only the geneaological lines [see last side of (1.9)] which move from the minimum or end maximum of the x_i can hit the boundary because the factor of antisymmetry annihilates the crossing genealogical lines. We know that a trajectory of a process with creation can branch as a consequence of the definition (see Ref. 8) only when it hits the boundary of Λ: In this case it is possible not to consider the branching of those trajectories which come from intermediate (not extremal) points because they do not give a contribution to the integral. Now we can majorize (1.9) in the following way: Remove the interdiction of crossing to the genealogical lines corresponding to extrema of (x_i). (This is a majorization because the set of trajectories which form the integration set, is widened.)

Now taking account of the previous observation, we can majorize (1.9) in the following way: We remove for the trajectories descending from the two extremal points the condition of not intersecting and minorize their interaction with the other particles. In this way we get majorization of (1.9) in which the contribution of extremal trajectories is factorized whereas the contribution of the remaining trajectories can be evaluated by means of the measure $P^{\infty}_{x,y}$ (that is the conditional Wiener measure with absorption on the boundary). We therefore obtain

$$\frac{1}{N!}\int_{\Lambda^N}P^k_{(x^N),(y^N)}\alpha(\bar{\omega})\exp[-U_N(\bar{\omega})]d(x^N)$$

$$=\int_{x_1<x_2<\cdots<x_N}P^k_{(x^N,x^N)}(d\omega^N\alpha(\bar{\omega})$$

$$\times\exp[-U_N(\bar{\omega})]d(x^N)$$

$$\leqslant\left(\int P^k_{xx}dx\right)^2e^{\beta C}\frac{1}{(N-2)!}\int_{\Lambda^{N-2}}P^{\infty}_{(x^{N-2})(x^{N-2})}(d\omega^{N-2})$$

$$\times\exp\left[-\int_0^{\beta}[U_{N-2}(\omega^{N-2}(t))]\right.$$

$$\left.+2\tilde{W}(\bar{\omega}^{N-2}(t))dt\right]dx^{N-2}, \tag{2.4}$$

where we set $\tilde{W}(x_1,\ldots,x_{N-2})=\inf_s[\Sigma_i\Phi(x_i-s)]$ to minorize the interaction of the internal particles with the extremal ones. Using the initial remark, (2.4) can be majorized by

$$|\Lambda|^2Q^2\frac{1}{(N-2)!}\int_{\Lambda^{N-2}}P^{\infty}_{(x^{N-2}),(x^{N-2})}(d\omega^{N-2})$$

$$\times\exp\left[-\int_0^{\beta}\{U_{N-2}(\omega^{N-2}(t))\right.$$

$$\left.+2\tilde{W}(\omega^{N-2}(t))\}dt\right]=\alpha_{\Lambda}(\omega^{N-2})d(x)^{N-2}. \tag{2.5}$$

Our goal is to show that the contribution of the term $\tilde{W}(\bar{\omega}^{N-2}(t))$ to the free energy becomes negligible in the limit $|\Lambda|\to\infty$. Given a constant $d>0$, we divide Λ into intervals $\Delta_1,\Delta_2,\cdots,\Delta_{[|\Lambda|/d]+1}$ of length d, with the exception of the last one, whose length is $|\Lambda|-d[|\Lambda|/d]$ and define the sequence $\{\alpha_N\}$ as $\alpha_N=[N/\log\log N]$.

We divide the set Λ^{N-2} into two subsets K_1 and K_2. If $x\in\Lambda^{N-2}$ and Δ_i is one of the intervals, we denote by $p(x,\Delta_i)$ the number of the components x_l of x such that $x_l\in\Delta_i$, and define

$$K_1\equiv\left\{x\in\Lambda^{N-2}\ \text{s.t. for}\ i=1,\ldots,\left[\frac{|\Lambda|}{d}\right]+1, p(x,\Delta_i)\leqslant\alpha_N\right\},$$

$$K_2\equiv\Lambda^{N-2}\setminus K_1.$$

We evaluate the Lebesgue's measure of K_2. This measure is equal to the probability that a point x, with uniform distribution in Λ^{N-2} belongs to K_2 times $|\Lambda|^{N-2}$. This

probability is less than a constant times the probability of the same event computed from a Poisson process distribution in the interval Λ, with the mean $\lambda > C(N-2)$, where C is a constant $C > 1$.[10] Given a Λ_i, we have

$$P\{p(x,\Delta_i > \alpha_N\}$$

$$\leqslant \sum_{k=\alpha_N}^{+\infty} \left(\frac{CN}{2N/\rho d}\right)^k \frac{1}{k!} \exp\left(\frac{-CN}{2N/\rho d}\right)$$

$$\leqslant C^1 \frac{1}{\alpha_N!} (2C\rho d)^{\alpha_N} e^{-2C\rho d} \tag{2.6}$$

and therefore

$$\text{meas} K_2 \leqslant \frac{N}{\rho d} \frac{C'(C\rho d)^{N/\log\log N}}{[(N/\log\log N)]!} e^{-C\rho d} |\Lambda|^{N-2}. \tag{2.7}$$

For what concerns the trajectories with initial and final points in K_1, we divide the space Ω of the N *tuples* of trajectories, not intersecting each other with initial and final points in K_1 into two subsets Ω_1 and Ω_2. If $\{\beta_N\}$ is the sequence $\{\beta_N\} = \{[N/\log\log\log N]\}$,

$$\Omega_1 \equiv \{\bar{\omega} \in \Omega / \forall t \in [0,\beta], \quad \text{for } i = 1,\ldots,[|\Lambda|/d]+1,$$

$$p(\bar{\omega}(t),\Delta_i) \leqslant \beta_N\}, \ \Omega_2 = \Omega \setminus \Omega_1.$$

We want to majorize $P_{xx}^{(\infty)}(\Omega_2)$ uniformly for $x \in K_1$. The event Ω_2 can be written as

$$\Omega_2 = \bigcup_{i=1}^{|\Lambda|+1} E_i,$$

where $E_i = \{\bar{\omega} \in \Omega \mid \exists t \in [0,\beta], p(\bar{\omega}(t), \Lambda_i) > \beta_N\}$.

We majorize $P_{xx}^{(\infty)}(E_i)$; for the sake of simplicity we take $i = 1$ without losing generality. Because of the condition of not intersecting, the event E_1 is equivalent to the event that the trajectories starting from the first β_N points reach Δ_1 for some $t \in [0,\beta]$. So we consider the probability of the last event. We majorize this probability in the following way:

(a) we remove the condition of not intersecting and remaining in Λ for $t \in [0,\beta]$;

(b) the particles can reach Δ_1, each one at a different instant and are not requested to be together in Δ_1;

(c) the starting points of the β_N trajectories are located in the nearest position to Δ_1 with the condition that $x \in K_1$, that is, there are α_N starting points at each of the left end points of the first $[\beta_N/\alpha_N]$ intervals;

(d) we majorize the probability of reaching Δ_1 for trajectories starting from $\Delta_3, \Delta_4, \ldots, \Delta_{\beta_N/\alpha_N}$ with that for a free (not conditioned) Brownian motion, which is surely correct for d big enough.

We obtain in this way

$$P_{xx}^{\infty}(E_1)$$

$$\leqslant \prod_{j=1}^{[\beta_N/\alpha_N]-2} \left[\frac{\sqrt{\beta}}{\sqrt{2\pi j\gamma}} e^{-(jd)^2/4\beta}\right]^{\alpha_N}$$

$$\leqslant \exp\left[-\gamma \frac{N(\log\log N)^2}{(\log\log\log N)^3}\right] \quad \forall \ x \in k_1, \tag{2.8}$$

where γ is a suitable constant, and we use the distribution of the minimum of a free Brownian motion and the usual estimate for the tail of the normal distribution. Therefore,

$$P_x(\Omega_2)$$

$$\leqslant \sum_{i=1}^{[|\Lambda|/d]} P(E_i)$$

$$\leqslant \exp\left[-\gamma \frac{N(\log\log N)^2}{(\log\log\log N)^3} + \log\left(\frac{2N}{\rho d}\right)\right]. \tag{2.9}$$

Now the integral of the formula (2.5) can be estimated in the following way

$$(2.5) \leqslant |\Lambda|^2 Q^2 e^{\beta C} \frac{1}{(N-2)!}$$

$$\times \left(\int_{K_1} d(x^{n-2}) \int_{\Omega_1} dP_{x^{N-2}}^{\infty}(\omega^{N-2})\right.$$

$$\times \exp\left\{-\int_0^{\beta} [U(\omega^{N-2}(t)) + 2\tilde{W}(\omega^{N-2}(t)))]dt\right\}$$

$$\left. + \int_{K_1} d(x^{N-2}) \int_{\Omega_2} + \int_{K_1} dx^{N-2} \int_{\Omega}\right). \tag{2.10}$$

Since in the first term of the sum ω^{N-2} is in Ω_1, $\tilde{W}(\omega^{N-2}(t))$ is minorated by $KN/\log\log\log N \ \forall \ t \in [0,\beta]$, where K is a suitable constant. Using (2.7) and (2.9) we obtain

$$(2.10) \leqslant |\Lambda|^2 \frac{Q^2 e^{sC}}{(N-2!)} e^{\beta KN/\log\log\log N}$$

$$\times \int_{\Lambda^{N-2}} dx^{N-2} \int_{\Omega} dP^{\infty}(\omega^{N-2})$$

$$\times \exp\left[-\int_0^{\beta} U(\omega^{N-2}(t))dt\right] + \frac{2^{N-2}N^{N-2}}{\rho^{N-2}}$$

$$\times \exp\left\{-N\gamma \frac{(\log\log N)^2}{(\log\log\log N)^3}\right.$$

$$\left. + \log\left(\frac{2N}{\rho d}\right)\right\} e^{\beta B(N-2)}$$

$$+ e^{\beta B(N-2)} \frac{2N}{\rho d} \frac{C'(C\rho d)^{(N/\log\log N)}}{[N/\log\log N]!}$$

$$\times e^{-c\rho d} \left(\frac{2N}{\rho}\right)^{N-2}. \tag{2.11}$$

The trace of $\exp(-\beta H^{\infty}_{N-2})$ appears in the first term of the sum. Therefore,

$$\lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \sup \frac{1}{\beta}\frac{\log Z^{k}(\Lambda,\beta,N)}{|\Lambda|} \leqslant \lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \sup \frac{1}{\beta}\frac{\log Z^{\infty}(\Delta,\beta,N)}{|\Lambda|}, \tag{2.12}$$

since the other terms do not contribute to the lim sup. On the other hand, the integral for the process with creation ($k<0$) is made over a bigger set of trajectories than for the process with absorption, whereas the proabability measure is equal in the common part of the two sets. Therefore, we have

$$\lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \inf \frac{1}{\beta}\frac{\log Z^{k}(\Lambda,\beta,N)}{|\Lambda|} \geqslant \lim_{\substack{|\Lambda|\to\infty \\ N/|\Lambda|\to\rho}} \inf \frac{\log Z^{\infty}(\Lambda,\beta,N)}{|\Lambda|}. \tag{2.13}$$

And the inequalities (2.12) and (2.13) imply the theorem.

APPENDIX

We call v-dimensional Brownian motion with initial point x a stochastic process
Borel subjects of $\mathbb{R}^{v}$ and $0<t_1<t_2<\cdots<t_n$

$$P(x_{t_1}\in B_1, x_{t_2}\in B_2,\ldots,x_{t_n}\in B_n) = \int\int\cdots\int \psi_{t_1}(x_1-x)\,\psi_{t_2-t_1}(x_2-x_1)\cdots\psi_{t_n-t_{n-1}} \times(x_n-x_{n-1})dx_1\cdots dx_n, \tag{A1}$$

where

$$\psi_t(x)=\frac{1}{(\sqrt{2\pi t})^{v}}\exp\left(-\frac{1}{2}\frac{|x|^2}{t}\right). \tag{A2}$$

It is known (see, for example, Ref. 11) that there are realizations of the Brownian motions [i.e., $\mathcal{F}$measurable maps from a suitable probability space $(\Omega, \mathcal{F}, P)$ into the paths in $\mathbb{R}^{v}$ such that (A1) is verified] such that the trajectory is continuous with proability 1. P is called Wiener measure.

We note that the function (A2) is the Green's function of the heat equation defined on the whole space $\mathbb{R}^{v}$;

$$\frac{\partial u}{\partial t}=\frac{1}{2}\Delta u. \tag{A3}$$

Therefore, the solution of the heat equation with initial condition $u(0,x)=f(x)$, $x\in\mathbb{R}^{v}$ can be expressed in terms of a Brownian motion in the form

$$u(t,x)=E_x[f(\omega(t))], \tag{A4}$$

where E_x denotes the expectation (A2) with respect to the Wiener measure with initial point x, and ω is the sample path.

In other words, the operator $e^{t\Delta}$ can be expressed through the Wiener integral.

If we consider the heat equation on a bounded region D, the solution depends on the boundary conditions that we impose. From the point of view of the Wiener integral, this leads us to consider processes whose behavior is different from that of the free Brownian motion only at the instants when the trajectories touch the boundary of D. Let us examine the case of the paper, whose study has been carried out in detail and in greater generality in Ref. 8, that is, the boundary conditions with $k<0$, and $\partial/\partial n$ denotes the inward nor mal derivative. For this paper is is sufficient to consider the case when D is an interval. In this case it is easy to define the reflected Brownian motion. If $x\in D$ we define the map $p:\mathbb{R}\to D$,

$$p(x)=x-2nL \quad \text{if} \quad (2n-\tfrac{1}{2})L\leqslant x\leqslant(2n+\tfrac{1}{2})L,$$

$$p(x)=(2n+1)L-x \quad \text{if} \quad (2n+\tfrac{1}{2})L\leqslant x\leqslant(2n+\frac{3}{2})L.$$

If $\omega(t)$ is a continuous trajectory $\omega:[0,\infty]\to\mathbb{R}$ $p(\omega(t))$ is a continuous trajectory in D and the process

$$\Omega\to p(\omega(t))$$

is called reflected Brownian motion.

The reflected Brownian motion corresponds to the boundary condition $\partial u/\partial n=0$ in the end points of the interval.

In order to obtain the process corresponding to the boundary condition $\partial u/\partial n=ku$ with $k<0$ it is natural to think that for this process not only the trajectories must be reflected by the boundary but new particles must be created. The creation of particles must depend on the time spent by the first particle in the points of the boundary. A measure of this time is given by the local time.

If a is one of the end points of D we say that $\bar{t}_a(\omega,t)$ is the local time that the trajectory ω has spent in a until the instant t if

$$\bar{t}_a(\omega,t)=\lim_{\epsilon\to 0}\frac{1}{2\epsilon}\operatorname{meas}\{s\,|\,0\leqslant s\leqslant t,\ |\omega(s)-a|<\epsilon\}$$

where the measure appearing in the definition is the usual Lebesque measure.

There are realizations of the Brownian motion for which the limit in (A5) exists with probability 1 (see Ref. 12).

We can now construct the stochastic process corresponding to the boundary conditions $\partial u/\partial n=ku$ with $k<0$. We give the initial trajectory the diadical index $\frac{1}{2}$ and associate to it the local time $\bar{t}_{\partial D}(\omega_{1/2},t)$ spent on the boundary of D, defined as the sum of the local times spent in the end points until the instant t. By enlarging the probability space we define a random variable $m_{1/2}$ distributed according to the law

$$P(m_{1/2}\geqslant t/\mathcal{F}_t)=\exp[k\bar{t}_{\partial D}(\omega_{1/2},t)],$$

where $\mathcal{F}_t$ is the σ-algebra generated by the events $\{\omega(s)\in A\}$, $0\leqslant s<t$.

It is easy to see that with probability 1, $\omega_{1/2}(m_{1/2})\in\partial D$, since

the local time increases only when the particle touches one of the two end points of D. At the instant $m_{1/2}$ the initial particle dies and is replaced by two particles that start their motion from the point $\omega_{1/2}(m_{1/2})$, we give them the indices $\frac{1}{4}$ and $\frac{3}{4}$ and define two random variables $m_{1/4}$ and $m_{3/4}$ in a larger probability space, with distribution as in (A6), at the instants $m_{1/4}$ and $m_{3/4}$ the particles split in two, and so on.

The solution of the Eq. (3) with boundary conditions $(\partial u/\partial n)\mid_{\partial D} = ku,\ k<0$ and initial condition $u(0,x)=f(x)$ can then be written as

$$u(x,t)=E_x\left[\sum_{i\in J_t} f(\omega_i(t))\right]$$

where the expectation is taken with respect to the process that we have described, and J_t is the set of the indices of the particles present at the instant t.

So we have constructed the operator $e^{t\Delta}$ where Δ is the self-adjoint extension of the operator $\partial^2/\partial x^2$ defined on the functions $C^2(D)$ which verifies

$$\left|\frac{\partial u}{\partial x}\right|_{\partial D} = ku.$$

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Addendum: On the inverse problem of transport theory with azimuthal dependence [J. Math. Phys. 19, 994 (1978)]

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A simplified expression is given for the moments over all space and angle of the intensity arising from an azimuthally-dependent plane source in an infinite medium. This provides a convenient equation for evaluating the mean of even powers of distance of travel of particles.

For a plane source in an infinite medium, the radiation intensity $I(\tau, \mu, \phi)$ depends only upon the spatial coordinate τ, the cosine of the polar angle, μ, and the azimuthal angle ϕ. Moments of this distribution $K^m_{l,n}$ for non-negative integers l, m, n may be defined as

$$K^m_{l,n} = \int_{-\infty}^{\infty} d\tau\, \tau^n \int_0^{2\pi} d\phi \cos m\phi \int_{-1}^{1} d\mu\, P^m_l(\mu) I(\tau, \mu, \phi), \tag{1}$$

where $P^m_l(\mu)$ is the associated Legendre polynomial. Symmetry considerations reveal that $K^m_{l,n} = 0$ for $(n + l + m)$ odd and for $n < (l - m)$.

The moments of Eq. (1) also may be expressed in terms of the Fourier expansion coefficients $I^m(\tau, \mu)$ as

$$K^m_{l,n} = 2\pi \int_{-\infty}^{\infty} d\tau\, \tau^n \int_{-1}^{1} dm(\mu) p^m_l(\mu) I^m(\tau, \mu), \tag{2}$$

where the notation is that of Ref. 1. The moments are a function only of μ_0, the cosine of the polar angle of the source radiation, and the parameters

$$h_l = 2l + 1 - \bar{\omega}_l. \tag{3}$$

The $\bar{\omega}_l$, $1 \le l \le N$, are the Legendre expansion coefficients describing the anisotropy of scattering of the medium, while for the isotropic term $\bar{\omega}_0 < 1$ since some absorption is assumed. The assumption of finite scattering order N leads to an additional condition that $K^m_{l,n} = 0$ for $m > N$.

The general result for the $K^m_{l,n}$ derived in Ref. 1 can be simplified by generalizing a result of Cacuci and Goldstein,[2] who provided an elegant expression for $K^0_{0,n}$ as a part of their investigation of neutrons slowing down in an infinite medium of constant cross section. The general result is

$$K^m_{l,n} = K^m_{l,l-m} \frac{n!}{(l-m)!} \sum_{j_0=0}^{l-m} w_{j_0} \sum_{j_1=0}^{j_0+1} w_{j_1} \sum_{j_2=0}^{j_1+1} w_{j_2} \cdots \times \sum_{j_{(n+m-l-2)/2}=0}^{j_{[(n+m-l-4)/2]+1}} w_{j_{(n+m-l-2)/2}}, \tag{4}$$

where the w's depend upon m and are defined as

$$w_j = (j+1)(2m+j+1)/(h_{j+m} h_{j+m+1}). \tag{5}$$

The values of $K^m_{l,l-m}$ in the right-hand side of Eq. (4) are given by

$$K^m_{l,l-m} = K^m_{m,0} (l-m)!\ (l+m)! \prod_{n=1}^{l-m} \frac{1}{h_{n+m}}, \quad l > m, \tag{6}$$

where

$$K^m_{m,0} = (1 - \mu_0^2)^{m/2} (2m+1)!!/h_m. \tag{7}$$

Equation (4) eliminates the need for evaluating a determinant, as in Ref. 1, to obtain $K^m_{l,n}$.

The use of Eq. (4) leads to a general equation for the mean of even powers of the distance of travel of particles in the mth azimuthal mode, which is defined by

$$\langle \tau^{2n} \rangle_m = K^m_{m,2n} / K^m_{m,0}. \tag{8}$$

The result is

$$\langle \tau^{2n} \rangle_m = (2n)! \sum_{j_0=0}^{0} w_{j_0} \sum_{j_1=0}^{j_0+1} w_{j_1} \sum_{j_2=0}^{j_1+1} w_{j_2} \cdots \times \sum_{j_{(n-1)}=0}^{j_{(n-2)}+1} w_{j_{(n-1)}} \tag{9}$$

The nested sum in the right-hand side of Eq. (9) is identical in form to ratios of the "eigenvalue space" moments calculated by Cacuci and Goldstein, except that the w's are now defined for any m. Explicit expressions for this sum for $n \le 18$ are available.[2]

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ERRATA

Erratum: On the positivity of energy in general relativity [J. Math. Phys. 19, 1152 (1978)]

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Equation (25) should read,

$$\frac{df(t)}{dt} = -\int \bar{\phi} D_a[(\bar{\pi}+v)^2 \bar{\gamma}^a] d\bar{A}$$

$$= -\tfrac{1}{2}\int \bar{\phi}(\bar{\pi}+v)[2\bar{\Omega} - (\bar{\pi}+v)^2] d\bar{A}$$
$$+ 2\int \bar{\phi}(\bar{\pi}+v)[(\mu - K^{-1/2} J^a D_a w) + \tfrac{1}{2}(\bar{\pi}^{ab}\bar{\pi}_{ab} - \tfrac{1}{2}\bar{\pi}^2)$$
$$+ \bar{\partial}_a T^a + \bar{\phi}^{-1}\bar{\partial}^a\bar{\partial}_a\bar{\phi} - \bar{\phi}^{-1} T^a \bar{\partial}_a\bar{\phi}] d\bar{A}$$
$$+ \int \bar{\phi}(\bar{\pi}+v)[\bar{p}^{ab}\bar{p}^{cd} q_{ac} q_{bd} - (\bar{p}^{ab} q_{ab})^2 - \tfrac{1}{2} v^2] d\bar{A}.$$

Equation (27) should read,

$$\frac{df(t)}{dt} = -\tfrac{1}{2} f(t) + 2\int [(\mu - K^{-1/2} J^a D_a w)$$
$$+ \tfrac{1}{2}(\bar{\pi}^{ab}\bar{\pi}_{ab} - \tfrac{1}{2}\bar{\pi}^2) + \bar{\partial}_a T^a + \bar{\partial}_a(\bar{\phi}^{-1}\bar{\partial}^a\bar{\phi})] d\bar{A}$$
$$+ \int [\bar{p}^{ab}\bar{p}^{cd} q_{ac} q_{bd} - (\bar{p}^{ab} q_{ab})^2 - \tfrac{1}{2} v^2 - 2\bar{\phi}^{-1} T^a \partial_a\bar{\phi}$$
$$+ 2\bar{\phi}^{-2}\bar{\partial}_a\bar{\phi}\partial^a\bar{\phi}] d\bar{A} \geq -f(t) + \int [\bar{p}^{ab}\bar{p}^{cd} q_{ac} q_{bd} - (\bar{p}^{ab} q_{ab})^2$$
$$- \tfrac{1}{2} v^2 - 2\bar{\phi}^{-1} T^a \bar{\partial}_a\bar{\phi} + 2\bar{\phi}^{-2}\bar{\partial}_a\bar{\phi}\bar{\partial}^a\bar{\phi}] d\bar{A}.$$

Equation (30) should read,

$$\int [\bar{p}^{ab}\bar{p}^{cd} q_{ac} q_{bd} - (\bar{p}^{ab} q_{ab})^2 - \tfrac{1}{2} v^2 - 2\bar{\phi}^{-1} T^a \bar{\partial}_a\bar{\phi} + 2\bar{\phi}^{-2}\bar{\partial}_a\bar{\phi}\bar{\partial}^a\bar{\phi}] d\bar{A}$$
$$= \int [\beta^a \beta_a (\tfrac{1}{2} - \tfrac{1}{8} K^{-1} D_n w D_m w q^{mn}) + (\gamma^{ab}\gamma_{ab} - \tfrac{1}{2}\gamma^2)$$
$$+ \tfrac{1}{2}(T^a - 2\bar{\phi}^{-1}\bar{\partial}^a\bar{\phi})(T^b - 2\bar{\phi}^{-1}\bar{\partial}^a\bar{\phi})\bar{q}_{ab} + \tfrac{3}{2} K^{-1}\alpha^2] d\bar{A} \geq 0.$$

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