Homothetic motions and the Hauser metric

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The Hauser metric is found in the canonical form obtained by Halford for a vacuum metric of Petrov type N admitting a two parameter group of homothetic motions. A result concerning the symmetries of vacuum metrics of Petrov type N possessing twisting geodesic rays is corrected.

1. INTRODUCTION

Vacuum metrics of Petrov type N are generated by a complex function $\Omega = \Omega(\zeta, \bar{\zeta}, u)$ satisfying the two field equations

$$\bar{D}\partial_u D\Omega = 0 \tag{1.1}$$

and

$$\bar{D}\bar{D}D\Omega - DD\bar{D}\bar{\Omega} = 0, \tag{1.2}$$

where the bar denotes complex conjugation and the operator D is defined by

$$D = \partial_\zeta - \Omega\partial_u . \tag{1.3}$$

In a recent article[1] Halford has shown that if such a metric admits a two parameter group of homothetic motions, then the coordinates can be chosen so that the function Ω takes one of the canonical forms

$$\text{(i)} \quad \Omega = y^{-1} f(u), \tag{1.4}$$

$$\text{(ii)} \quad \Omega = u^{a/(a+1)} g(y^{a+1}/u), \quad \text{with } a \neq -1 . \tag{1.5}$$

Here $y = (\zeta - \bar{\zeta})/2i$. In particular the Hauser metric[2] is known to possess such a group but Halford states that it remains to extract the Hauser metric from the Eqs. (1.1)–(1.5). In Sec. 2 it is shown that the Hauser metric corresponds to $a = 5/2$.

In 1969 the present author[3] considered the symmetries of vacuum metrics of Petrov type N possessing twisting geodesic rays but, as Leroy points out in his paper[4] on the group of conformal motions admitted by such metrics, the conclusions drawn were, in fact, incorrect. In Ref. 3 I proved that if a Killing vector exists then the coordinates can be chosen so that the vector takes a particularly simple form and the function Ω then takes the canonical form

$$\Omega = \Omega(\zeta + \bar{\zeta}, u). \tag{1.6}$$

I found that only one Killing vector can exist having the simple form referred to above and concluded that only one symmetry exists. This conclusion is false; if more than one Killing vector exists then these vectors take the simple form *simultaneously* if and only if the corresponding group of motions is abelian. Hence the correct conclusion to be drawn from the working in Ref. 3 is

Theorem 1: A vacuum metric of Petrov type N with twisting geodesic rays cannot admit an abelian group of motions of order greater than one.

Using the canonical form (1.6) the author has now completed the integration of Killing's equations and also of the homothetic Killing's equations. This work is summarized in

Theorem 2: A vacuum metric of Petrov type N with twisting geodesic rays cannot admit a group of homothetic motions of order greater than two. If such a group exists then the coordinates can be chosen so that Ω takes the canonical form

$$\Omega = (\zeta + \bar{\zeta})^{-\beta} F(u(\zeta + \bar{\zeta})^{\beta - 1}), \tag{1.7}$$

and if the group reduces to a group of motions (i.e., the metric has two symmetries) then

$$\beta = 0. \tag{1.8}$$

The maximal order of the group has already been established by Halford and Leroy so the proof of the above theorem will not be given. Notice that under the transformation $\zeta \to i\zeta$ the two canonical forms (1.4) and (1.5) given by Halford reduce to the single form (1.7) with $a = -\beta$. Unfortunately Halford used the results given in Ref. 3 and so could not realize that the case $a = 0$ corresponds to the existence of two Killing vectors.

2. THE HAUSER METRIC

The Hauser metric, in the form given in Ref. 5, can be written in the notation used by Halford and the author by making

(i) a change of signature;

(ii) a coordinate transformation:

$$u = \tfrac{1}{2}\Delta_0(\zeta + \bar{\zeta})^{7/2} H(y), \quad r = \rho ,$$

with

$$H'(= dH/dy) = 2^{-3/4} f(y), \quad \text{where } y = 2\sigma/\Delta_0(\zeta + \bar{\zeta})^2 , \tag{2.1}$$

(iii) a null rotation leaving k invariant

$$k^* = k,$$

$$n^* = b - \bar{A}t - At - A\bar{A}k ,$$

$$t^* = t + \bar{A}k ;$$

(iv) the identification between the tetrads used by the different authors

$$1 \equiv -k^*,$$

$$n \equiv n^*,$$

$$m \equiv t^*.$$

The metric is then found to correspond to

$$\Omega = (\zeta + \bar{\zeta})^{5/2} \Delta_0 \left| H'(i + y) - \tfrac{7}{4} H \right| . \tag{2.2}$$

According to Eq. (2.1)

$$\tfrac{1}{2}\Delta_0 H(y) = u(\zeta + \bar{\zeta})^{-7/2}$$

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and this equation can, in principle, be inverted to give y as a function of $u(\zeta+\bar{\zeta})^{-7/2}$,

$$y = y(u(\zeta+\bar{\zeta})^{-7/2}) . \tag{2.3}$$

Then (2.2) can be rewritten as

$$\Omega = (\zeta+\bar{\zeta})^{5/2} F(u(\zeta+\bar{\zeta})^{-7/2}) , \tag{2.4}$$

where

$$F = 2(y')^{-1}(i+y) - \tfrac{7}{2} u(\zeta+\bar{\zeta})^{-7/2} , \tag{2.5}$$

the prime on y now denoting differentiation with respect to $u(\zeta+\bar{\zeta})^{-7/2}$. The form (2.4) corresponds to (1.7) with $\beta = -\frac{5}{2}$ [and therefore (1.5) with $a = \frac{5}{2}$]. The function y must satisfy the remaining Hauser field equation which becomes

$$-y'''y' + 3y''^2 + 3y'^4/16(1+y^2) = 0 . \tag{2.6}$$

It is natural to ask the question whether the Hauser metric can be generalized by taking Ω in the form (1.7) with

$$F = 2(y')^{-1}(i+y) + (\beta-1) u(\zeta+\bar{\zeta})^{\beta-1} ,$$

where

$$y = y(u(\zeta+\bar{\zeta})^{\beta-1}) .$$

In fact the field equation (1.1) can only be satisfied if $\beta = -\frac{5}{2}$ or -5 or -6. The case $\beta = -\frac{5}{2}$ leads to the Hauser metric and the remaining cases lead to the equation

$$y''y'^{-2}(1+y^2) + 2y = 0 .$$

Unfortunately $\bar{D}\bar{D}D\Omega - DD\bar{D}\bar{\Omega}$ is then a nonzero constant so that the field equation (1.2) cannot be satisfied.

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Multiple scattering theory for discrete, elastic, random media

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A theory is presented for determining the ensemble-averaged Green tensor of a statistically homogeneous distribution of identical, randomly oriented elastic scatterers embedded in an infinite, homogeneous, and isotropic matrix. The theory is based on the self-consistent formulation of Lax's [Rev. Mod. Phys. **23**, 287 (1951); Phys. Rev. **85**, 621 (1952)] multiple scattering theory due to Gyorffy [Phys. Rev. B **1**, 3290 (1970)] and Korringa and Mills [Phys. Rev. B **5**, 1654 (1972)]. The average Green tensor is found to be characterized by three parameters which may depend on the momentum operator but which are otherwise analogous to the Lamé constants and density of an ideal, homogeneous, and isotropic medium. These "effective" parameters are shown to be related in the usual way to the wave numbers of coherent compressional and shear plane-wave modes of the random composite. The ensemble averaged Green tensor and the *dispersion relations* satisfied by the wave numbers of the coherent modes are found to depend on the single and joint probability density functions for the scattering centers and on the transition operator of a discrete scatterer embedded in the effective (average) medium. The dispersion relations are evaluated explicitly for the limiting case of a completely random ensemble of homogeneous and isotropic scatterers whose elastic parameters and density differ very little from those of the matrix medium.

1. INTRODUCTION

In this paper a theory is developed for determining the ensemble-averaged Green tensor and effective elastic parameters and density of a random configuration of identical, randomly oriented elastic scatterers embedded in an inifinte homogeneous, isotropic elastic medium. The problem of calculating effective parameters for a random ensemble of discrete scatterers arises in a number of disciplines which include electromagnetic and acoustic wave propagation[1-8] and electron propagation in liquid metals and amorphous solids.[9-15] The probabilistic formulation of this problem employed in this paper has its origins in the pioneering works of Foldy[16] and Lax[8] which dealt primarily with determining the index of refraction of a statistically homogeneous ensemble of discrete scatterers. Probably the greatest advances in this problem in recent years have been in quantum mechanical applications[9-15] although the formalism developed in these works applies equally well to electromagnetic and acoustic wave propagation.

The problem addressed in this paper is somewhat more complex than the analogous quantum mechanical one in that the quantities with which one must work are tensors as opposed to scalars and the differential equation satisfied by Green tensor is not the simple Schrödinger equation of quantum mechanics. Fortunately, however, by recasting the equation of motion for the Green tensor into an integral equation it is possible to formulate the elastic problem to be completely analogous to the quantum mechanical liquid metal and amorphous solid problems for which a number of well developed theories[9-15] are available for calculating the mean Green function. It is then possible to apply these theories (suitably modified) to the problem under consideration here.

The derivation of the integral equation satisfied by the Green tensor is presented in Sec. 2. The derived equation is entirely analogous to the integral equation for scattering that arises in electromagnetic and quantum mechanical scattering.[17] In order to obtain a closer parallelism with quantum mechanical scattering an operator form of the integral equation is obtained which is the elastic counterpart of the Lippmann–Schwinger equation of quantum mechanics.[17] The original integral equation is then obtained from the operator equation by taking matrix elements of the latter equation in the coordinate representation.

The multiple scattering problem for composite elastic media is formulated and solved in Sec. 3. The Lippman–Schwinger equation satisfied by the Green tensor of the composite medium is formally solved by introducing a scattering or transition operator, which although being a second rank tensor, is completely analogous to the transition operator used in quantum mechanical scattering.[18] The ensemble averaged Green tensor is then determined *self-consistently* by requiring the ensemble averaged transition operator for the composite medium to vanish. The average Green tensor so determined is found to be diagonal in the momentum representation (i.e., in Fourier space) and to depend on three parameters which are analogous to the Lamé constants and density of a perfect homogeneous, isotropic medium but which, in general, depend on the momentum vector (i.e., spatial frequency vector). Thus, although the average Green tensor characterizes a homogeneous and isotropic medium, this "average" medium is *spatially* dispersive[19] and hence may possess a number of longitudinal and/or transverse wave numbers.

The calculation of the ensemble average transition operator is the central problem addressed in discrete multiple scattering theory and the problem for which a number of

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approximate solution are available.[9-15] The approach adopted in Sec. 3 is to use the self-consistent form of the *quasicrystalline approximation* (QCA) initially developed for finite systems by Gyorffy[9] and later extended to infinite systems by Korringa and Mills.[10] The average Green tensor the results from the calculation is found to depend on the average number of scattering centers per unit volume (assumed constant), on the conditional probability distribution for a scattering center to be located at $\mathbf{r}$ given that one is located at $\mathbf{r}_0$ (assumed to depend only on $|\mathbf{r}-\mathbf{r}_0|$), and on the *single* scattering transition operator of a discrete scatterer *embedded in the average medium*. The computation of the average Green tensor requires the solution of three coupled, operator equations. In the special case of a completely random ensemble of scattering centers the result reduces to the elastic version of the coherent potential approximation (CPA).[20]

Section 4 is devoted to the derivation of the dispersion relations satisfied by the wave numbers of the coherent compressional and shear plane-wave modes of the random composite. It is shown that when correlations in scatterer locations can be ignored these dispersion relations can be expressed in terms of the forward compressional and shear wave *scattering amplitudes* of a single scatterer embedded in the effective medium. These scattering amplitudes have been approximately evaluated in the literature[21] for various scatterer shapes so that the derived dispersion relations can be readily evaluated for a number of cases of practical importance.

The final part of Sec. 4 is devoted to the approximate calculation of the wave numbers of the coherent modes when the composite medium consists of a completely random distribution of very weak, homogeneous and isotropic scatterers. For this case the Born approximation to the forward scattering amplitudes is used and one finds that the effective elastic parameters and density of the random composite are simply the volume weighted average values of those of the constituent phases. This simple example is intended only to be illustrative of the theoretical model developed in Sec. 3. A more realistic application of the theory will be presented elsewhere.

Theories for calculating effective elastic parameters for composite media are not scarce.[6,7,22-32] One of the earliest such investigations *based on scattering theory* is due to Herzfeld[7] who applied theories due to Lord Rayleigh[1] and Ewald[33] to the problem of calculating the velocity of sound in suspensions. Herzfeld's work is of interest here since his calculation based on Ewald's theory can be considered to be a certain limiting case of Lax's (non-self-consistent) QCA. More recent applications of the non-self-consistent QCA to multiple scattering of elastic waves in discrete random media are due to Varadan *et al.*[25] and to Sobszyk.[26] Zeller and Dederichs[31] and Gubernatis and Krumhansl[32] applied the CPA to the calculation of the effective parameters of composite elastic media in the static limit (i.e., for the zero frequency case). These latter two studies most resemble the work reported here in that they both employ the operator formalism of quantum mechanics and base their work on the Lippman–Schwinger equation obeyed by the strain tensor in the static limit. Thus, the work reported here can be considered to be a generalization of these studies to the nonstatic case, where, in addition, we account for short range correlation in the random media by employing the QCA as opposed to the CPA.

2. DERIVATION OF THE INTEGRAL EQUATION FOR SCATTERING

We consider an infinite, elastic medium having an elastic moduli tensor[34] C_{ijkl} and density ρ. A harmonically oscillating body force

$$\mathscr{S}_i(\mathbf{r}'',t) = S_i(\mathbf{r}'')e^{-i\omega t} \tag{2.1}$$

acting on this medium will generate a displacement field

$$\mathscr{U}_i(\mathbf{r}'',t) = u_i(\mathbf{r}'')e^{-i\omega t}, \tag{2.2}$$

whose amplitude $u_i(\mathbf{r}'')$ obeys the partial differential equation[35]

$$[C_{ijkl}(\mathbf{r}'')u_{k,l}(\mathbf{r}'')]_{,j} + \omega^2\rho(\mathbf{r}'')u_i(\mathbf{r}'') = S_i(\mathbf{r}''). \tag{2.3}$$

Equation (2.3) is formally solved by introducing a Green tensor $g_{im}(\mathbf{r}'',\mathbf{r})$ which satisfies Eqs. (2.3) for the case when the body force is the tensor $\delta_{im}\delta(\mathbf{r}''-\mathbf{r})$ with $\delta(\mathbf{r}''-\mathbf{r})$ being Dirac's delta function and δ_{im} the Kronecker delta function. Thus g_{im} satisfies the equation

$$[C_{ijkl}(\mathbf{r}'')g_{km,l}(\mathbf{r}'',\mathbf{r})]_{,j} + \omega^2\rho(\mathbf{r}'')g_{im}(\mathbf{r}'',\mathbf{r}) = \delta_{im}\delta(\mathbf{r}''-\mathbf{r}) \tag{2.4}$$

and appropriate boundary conditions at infinity.

By choosing the boundary condition at infinity satisfied by g_{im} to be Sommerfeld's radiation condition[36] we find that the solution to Eq. (2.3) can be expressed in the form

$$u_m(\mathbf{r}) = \int d^3r''\, g_{im}(\mathbf{r}'',\mathbf{r})S_i(\mathbf{r}''), \tag{2.5}$$

where the integration in Eq. (2.5) is over all space. The problem of solving Eq. (2.3) has thus been transformed to that of solving Eq. (2.4) subject to Sommerfeld's radiation condition.

Closed form solutions to Eq. (2.4) are known for only a few special cases. One case of considerable practical importance is that of a *homogeneous, isotropic* medium. For such a medium the density ρ^e is a constant and the elastic moduli tensor is of the form[35]

$$C^e_{ijkl} = \lambda^e\delta_{ij}\delta_{kl} + \mu^e(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{2.6}$$

where the parameters λ^e and μ^e are constants[37] (the Lamé constants). Because the elastic moduli tensor C^e_{ijkl} is independent of position the Green tensor G_{im} of a homogeneous, isotropic medium satisfies the equation

$$C^e_{ijkl}G_{km,lj}(\mathbf{r}-\mathbf{r}'') + \omega^2\rho^eG_{im}(\mathbf{r}-\mathbf{r}'') = \delta_{im}\delta(\mathbf{r}-\mathbf{r}''), \tag{2.7}$$

where the derivatives are with respect to the $\mathbf{r}''$ coordinates and where we have used the fact that G_{im} is a function only of the difference between the two position vectors $\mathbf{r}$ and $\mathbf{r}''$.

Many types of elastic media consist of a homogeneous, isotropic matrix in which are embedded one or more inclusions (elastic inhomogeneities). For such media the elastic moduli tensor C_{ijkl} and density ρ can be decomposed in the form

$$C_{ijkl} = C^e_{ijkl} + \Delta C_{ijkl}, \tag{2.8a}$$

$$\rho = \rho^e + \Delta\rho, \tag{2.8b}$$

where the Green tensor G_{im} associated with C^e_{ijkl} and ρ^e obeys Eq. (2.7). On substituting Eqs. (2.8) into Eq. (2.4), we find that $g_{im'}$ satisfies the equation

$$C^e_{ijkl}g_{km',lj}(\mathbf{r}'',\mathbf{r}') + \omega^2\rho^e g_{im'}(\mathbf{r}'',\mathbf{r}') = S_{im'}(\mathbf{r}'',\mathbf{r}'), \tag{2.9}$$

where the "source" $S_{im'}$ is given by

$$S_{im'}(\mathbf{r}'',\mathbf{r}') = \delta_{im'}\delta(\mathbf{r}''-\mathbf{r}') - \{[\Delta C_{ijkl}(\mathbf{r}'')g_{km',l}(\mathbf{r}'',\mathbf{r}')]_j + \omega^2\Delta\rho(\mathbf{r}'')g_{im}(\mathbf{r}'',\mathbf{r}')\}. \tag{2.10}$$

The solution to Eq. (2.9) that satisfies Sommerfield's radiation condition is given by Eq. (2.5) with g_{im} replaced by G_{im} and $S_i(\mathbf{r}'')$ by $S_{im'}(\mathbf{r}'',\mathbf{r}')$. We find that

$$\begin{aligned} g_{mm'}(\mathbf{r},\mathbf{r}') &= \int d^3r''\, G_{im}(\mathbf{r}-\mathbf{r}'')S_{im'}(\mathbf{r}'',\mathbf{r}') \\ &= G_{mm'}(\mathbf{r}-\mathbf{r}') - \int d^3r''\, G_{mi}(\mathbf{r}-\mathbf{r}'') \\ &\quad\times\{[\Delta C_{ijkl}(\mathbf{r}'')g_{km',l}(\mathbf{r}'',\mathbf{r}')]_j \\ &\quad + \omega^2\Delta\rho(\mathbf{r}'')g_{im'}(\mathbf{r}'',\mathbf{r}')\}, \end{aligned} \tag{2.11}$$

where we have used the fact that $G_{im} = G_{mi}$.

Equation (2.11) is an integral equation[38] obeyed by the Green tensor $g_{mm'}$ and is entirely equivalent to the partial differential equation (2.4) subject to Sommerfeld's radiation condition. The advantage of the integral equation over the differential equation is, for the purposes of this investigation, that Eq. (2.11) is very similar to the integral equation for scattering that forms the basis of much of the work in multiple scattering theory.[9-15] An even closer similarity results if we express this integral equation in operator form using the Dirac notation[39] employed in quantum mechanics. Within this formalism the integral equation is interpreted as being the equation satisfied by the matrix elements of an abstract operator[40] $\hat{g}_{mm'}$ defined on a linear vector space. The operator form of Eq. (2.11) is

$$\hat{g}_{mm'} = \hat{G}_{mm'} + \hat{G}_{mi}\Delta\hat{\Gamma}_{ik}\hat{g}_{km'}, \tag{2.12}$$

where

$$\Delta\hat{\Gamma}_{ik} = \hat{p}_j\Delta\hat{C}_{ijkl}\hat{p}_l - \omega^2\Delta\hat{\rho}\delta_{ik}, \tag{2.13}$$

and where $\hat{p}_j = -i\partial/\partial x_j$ is the usual momentum operator from quantum mechanics. The differential equation (2.7) can also be expressed in operator notation as follows:

$$\hat{\Gamma}^e_{ik}\hat{G}_{km} = -\delta_{im}\hat{I}. \tag{2.14}$$

Here $\hat{I}$ is the identity operator and

$$\hat{\Gamma}^e_{ik} = \hat{p}_j\hat{C}^e_{ijkl}\hat{p}_l - \omega^2\hat{\rho}^e\delta_{ik}, \tag{2.15}$$

with

$$\hat{C}^e_{ijkl} = \hat{\lambda}^e\delta_{ij}\delta_{kl} + \hat{\mu}^e(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{2.16}$$

On substituting Eq. (2.16) into Eq. (2.15) we find that $\hat{\Gamma}^e_{ik}$ can be expressed in terms of $\hat{\lambda}^e$, $\hat{\mu}^e$ and $\hat{\rho}^e$ as follows:

$$\hat{\Gamma}^e_{ik} = (\hat{\lambda}^e + 2\hat{\mu}^e)\hat{p}_i\hat{p}_k + \hat{\mu}^e(\hat{p}_j\hat{p}_j\delta_{ik} - \hat{p}_i\hat{p}_k) - \omega^2\hat{\rho}^e\delta_{ik}. \tag{2.17}$$

In deriving Eq. (2.17) we have made use of the fact that the operators $\hat{\lambda}^e$ and $\hat{\mu}^e$ commute with the momentum operator $\hat{p}_i$.

Equations (2.12) and (2.14) can be expressed in even more compact form using dyadic notation. In particular, was find that

$$\hat{\mathbf{g}} = \hat{\mathbf{G}} + \hat{\mathbf{G}}\cdot\Delta\hat{\Gamma}\cdot\hat{\mathbf{g}}, \tag{2.18a}$$

$$\hat{\Gamma}^e\cdot\hat{\mathbf{G}} = -\hat{\mathbf{I}}, \tag{2.18b}$$

where the tensors are recovered from the dyadics in the usual manner by taking the left and right dot products with appropriate unit vectors.[41]

Equation (2.18a) is the principle result of this section. This equation is entirely analogous to the Lippman–Schwinger equation[17] of quantum mechanical scattering and will form the basis for the theory presented in the following section.

3. MULTIPLE SCATTERING PROBLEM

We now consider an elastic medium whose elastic moduli tensor C_{ijkl} and density ρ are of the form

$$C_{ijkl}(\mathbf{r}) = C^0{}_{ijkl} + \sum_{n=1}^{N}\delta C^{(n)}_{ijkl}(\mathbf{r}), \tag{3.1a}$$

$$\rho(\mathbf{r}) = \rho^0 + \sum_{n=1}^{N}\delta\rho^{(n)}(\mathbf{r}), \tag{3.1b}$$

where $C^0{}_{ijkl}$ and ρ^0 characterize a homogeneous, isotropic medium, i.e.,

$$C^0{}_{ijkl} = \lambda^0\delta_{ij}\delta_{kl} + \mu^0(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{3.2}$$

with λ^0, μ^0 and ρ^0 being constants. The quantities $\delta C^{(n)}_{ijkl}$ and $\delta\rho^{(n)}$ characterize perturbations in the elastic medium which are caused by the presence of an inhomogeneity (scatterer) centered at the point $\mathbf{R}_n$. The scatterers are assumed to be identical in shape and composition, and to be randomly oriented in space.

The scattering centers $\{\mathbf{R}_n\}$ are assumed to be randomly distributed in accordance with the joint probability density function $P(\mathbf{R}_1,...,\mathbf{R}_N)$. The probability density function for a single scattering center (say $\mathbf{R}_1$) is given by

$$P(\mathbf{R}_1) = \int d^3R_2\cdots d^3R_N P(\mathbf{R}_1,...,\mathbf{R}_N) \tag{3.3}$$

and the joint probability density function for a pair of centers (say $\mathbf{R}_1,\mathbf{R}_2$) is

$$P(\mathbf{R}_1,\mathbf{R}_2) = \int d^3R_3\cdots d^3R_N P(\mathbf{R}_1,...,\mathbf{R}_N). \tag{3.4}$$

We will further assume that the scattering centers are uniformly distributed within a volume V; i.e.,

$$P(\mathbf{R}_1) = P(\mathbf{R}_2) = \cdots = P(\mathbf{R}_N) = \begin{cases} 1/V & \text{if } \mathbf{r} \text{ is contained in } V \\ 0 & \text{otherwise} \end{cases} \tag{3.5}$$

and the conditional density function

$$P(\mathbf{R}_2|\mathbf{R}_1) = P(\mathbf{R}_1,\mathbf{R}_2)/P(\mathbf{R}_1) \tag{3.6}$$

depends only on the distance $|\mathbf{R}_2 - \mathbf{R}_1|$ between the two centers.

We also introduce the quantity

$$\gamma(|\mathbf{R}_1 - \mathbf{R}_2|) = (N-1)P(\mathbf{R}_1|\mathbf{R}_2) - \bar{n}, \tag{3.7}$$

where $\bar{n} = NP(\mathbf{R})$ is the mean number of scatterers per unit volume. $\gamma(|\mathbf{R}_1 - \mathbf{R}_2|)$ is a measure of the *correlation* that exists between the scattering center locations $\mathbf{R}_1$ and $\mathbf{R}_2$. For a completely random ensemble the centers are statistically independent so that $P(\mathbf{R}_1|\mathbf{R}_2) = P(\mathbf{R}_1) = 1/V$ and Eq. (3.7) yields

$$\gamma_{\text{RANDOM}}(|\mathbf{R}_1 - \mathbf{R}_2|) = -1/V, \tag{3.8}$$

which becomes zero in the limit $V \to \infty$. The assumption of complete randomness is not realistic in most applications due to the intrinsic correlation that must exist to guarantee nonoverlap of the inhomogeneities $\delta C^{(n)}_{ijkl}$, $\delta\rho^{(n)}$ for different values of n.

The problem addressed in this section is the calculation of the ensemble average of the Green tensor for the elastic medium described above. The Green tensor for any particular realization of this discrete random medium satisfies Eq. (2.4) with C_{ijkl} and ρ given by Eqs. (3.1). The ensemble averaged Green tensor is then given by

$$\langle g_{im}(\mathbf{r}'',\mathbf{r})\rangle = \int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N) E\,[g_{im}(\mathbf{r}'',\mathbf{r})], \tag{3.9}$$

where $E\,[g_{im}]$ is the Green tensor averaged over all orientations of the scatterers for the realization $(\mathbf{R}_1,\ldots,\mathbf{R}_N)$ of the scattering centers.

As discussed in the Introduction, we shall adapt a procedure developed by Gyorffy[9] and Korringa and Mills[10] for quantum mechanical scattering problems to the present application. Toward this end we decompose the elastic moduli tensor C_{ijkl} and density ρ in the manner prescribed in Eq. (2.8) with C^e_{ijkl} being defined in Eq. (2.6) and with λ^e, μ^e and ρ^e being left, as yet, unspecified. The Green tensor $\hat{g}_{im}$ then satisfies the Lippmann–Schwinger equation [c.f., Eq. (2.12)]

$$\hat{g}_{im} = \hat{G}_{im} + \hat{G}_{ii'} \Delta\hat{\Gamma}_{i'k} \hat{g}_{km}, \tag{3.10}$$

with

$$\Delta\hat{\Gamma}_{i'k} = \sum_{n=1}^{N} \delta\hat{\Gamma}^{(n)}_{i'k} - \hat{W}_{i'k}, \tag{3.11}$$

where

$$\delta\hat{\Gamma}^{(n)}_{i'k} = \hat{p}_j \delta\hat{C}^{(n)}_{i'jkl} \hat{p}_l - \omega^2 \delta\hat{\rho}^{(n)} \delta_{i'k}, \tag{3.12a}$$

$$\hat{W}_{i'k} = \hat{\Gamma}^e_{i'k} - \hat{\Gamma}^0_{i'k}. \tag{3.12b}$$

$\hat{\Gamma}^e_{ik}$ is defined in Eqs. (2.15) and (2.17) and $\hat{\Gamma}^0_{ik}$ is given by these same expression with $\hat{C}^e_{ijkl}, \hat{\lambda}^e, \hat{\mu}^e$ and $\hat{\rho}^e$ replaced, respectively, by $C^0{}_{ijkl}, \lambda^0, \mu^0$ and ρ^0. Here $\delta\hat{C}^{(n)}_{i'jkl}$ and $\delta\hat{\rho}^{(n)}$ denote the operators whose matrix elements in the coordinate representation are

$$\langle \mathbf{r}|\delta\hat{C}^{(n)}_{i'jkl}|\mathbf{r}'\rangle = \delta C^{(n)}_{i'jkl}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'), \tag{3.13a}$$

$$\langle \mathbf{r}|\delta\hat{\rho}^{(n)}|\mathbf{r}'\rangle = \delta\rho^{(n)}(\mathbf{r})\delta(\mathbf{r}-\mathbf{r}'). \tag{3.13b}$$

We now introduce a *transition operator* $\hat{\mathscr{T}}_{i'k}$ defined, in analogy to the quantum mechanical transition operator,[18] by

$$\hat{\mathscr{T}}_{i'k} \hat{G}_{km} = \Delta\hat{\Gamma}_{i'k} \hat{g}_{km}. \tag{3.14}$$

On substituting Eq. (3.14) into Eq. (3.10) we obtain

$$\hat{g}_{im} = \hat{G}_{im} + \hat{G}_{ii'} \hat{\mathscr{T}}_{i'k} \hat{G}_{km}, \tag{3.15a}$$

or, in dyadic notation

$$\hat{\mathbf{g}} = \hat{\mathbf{G}} + \hat{\mathbf{G}} \cdot \hat{\mathscr{T}} \cdot \hat{\mathbf{G}}, \tag{3.15b}$$

where $\hat{\mathscr{T}}$ is the transition operator in dyadic notation.

Now the Green tensor $\hat{G}_{im}$, although at the moment unspecified, is a *nonrandom quantity*. Consequently, if we ensemble average both sides of Eq. (3.15b) we obtain

$$\langle \hat{\mathbf{g}} \rangle = \hat{\mathbf{G}} + \hat{\mathbf{G}} \cdot \langle \hat{\mathscr{T}} \rangle \cdot \hat{\mathbf{G}}, \tag{3.16}$$

where

$$\langle \hat{\mathscr{T}} \rangle = \int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N) E\,[\hat{\mathscr{T}}] \tag{3.17}$$

is the ensemble average of the transition operator. The problem of calculating the average Green tensor has thus been transformed into that of calculating the average transition operator.

It is easily verified using Eqs. (3.15b) and (3.14) that $\hat{\mathscr{T}}$ satisfies the operator equation

$$\hat{\mathscr{T}} = \Delta\hat{\Gamma} + \Delta\hat{\Gamma} \cdot \hat{\mathbf{G}} \cdot \hat{\mathscr{T}}, \tag{3.18}$$

where

$$\Delta\hat{\Gamma} = \sum_{n=1}^{N} \delta\hat{\Gamma}^{(n)} - \hat{\mathbf{W}}, \tag{3.19}$$

with $\delta\hat{\Gamma}^{(n)}$ and $\hat{\mathbf{W}}$ defined in tensor form in Eq. (3.12). It is apparent from Eq. (3.18) that $\hat{\mathscr{T}}$ depends on $\hat{\mathbf{G}}$ and, hence, on $\hat{\lambda}^e, \hat{\mu}^e$, and $\hat{\rho}^e$. Let us, for the moment assume that these quantities can be selected to be such that $\langle \hat{\mathscr{T}} \rangle = \mathbf{0}$.[42] In this event the second term on the right-hand side of Eq. (3.16) vanishes so that

$$\langle \hat{\mathbf{g}} \rangle = \hat{\mathbf{G}}. \tag{3.20}$$

The mean Green dyadic is thus given by the solution to Eq. (2.18b), viz.,

$$\hat{\mathbf{\Gamma}}^e \cdot \hat{\mathbf{G}} = -\hat{\mathbf{I}}, \tag{3.21}$$

where $\hat{\mathbf{\Gamma}}^e$ is defined in tensor form in Eq. (2.15) *with* $\hat{\lambda}^e, \hat{\mu}^e$ and $\hat{\rho}_e$ *being determined from the condition that the ensemble average of the transition operator vanish.*

The Green dyadic $\hat{\mathbf{G}}$ characterizes a *homogeneous, isotropic* medium and thus Eq. (3.16) will admit the solution $\langle \hat{\mathbf{g}} \rangle = \hat{\mathbf{G}}$ only if the random medium under consideration is statistically homogeneous and isotropic. Such is the case for the class of random media under consideration here due to our assumptions that 1) the orientation of any given scatterer is completely random, and 2) that the scattering centers are uniformly distributed with a conditional probability density function [defined in Eq. (3.6)] which depends only on the distance between the two scattering centers and not the direction of the vector joining these two centers.

Returning to Eq. (3.18) we substitute for $\Delta\hat{\Gamma}$ from Eq. (3.19) to obtain

$$\hat{\mathscr{T}} = \sum_{n=1}^{N} \hat{\mathbf{Q}}^{(n)} - \hat{\mathbf{q}}, \tag{3.22}$$

where $\hat{\mathbf{Q}}^{(n)}$ and $\hat{\mathbf{q}}$ are given by

$$\hat{\mathbf{Q}}^{(n)} = \delta\hat{\Gamma}^{(n)} + \delta\hat{\Gamma}^{(n)} \cdot \hat{\mathbf{G}} \cdot \hat{\mathscr{T}}, \tag{3.23a}$$

$$\hat{\mathbf{q}} = \hat{\mathbf{W}} + \hat{\mathbf{W}} \cdot \hat{\mathbf{G}} \cdot \hat{\mathscr{T}}, \tag{3.23b}$$

On taking the ensemble average of both sides of Eqs. (3.22) and (3.23b) we obtain

$$\langle \hat{\mathscr{T}} \rangle = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle - \langle \hat{\mathbf{q}} \rangle, \tag{3.24a}$$

$$\langle \hat{\mathbf{q}} \rangle = \hat{\mathbf{W}} + \hat{\mathbf{W}} \cdot \hat{\mathbf{G}} \cdot \langle \hat{\mathscr{T}} \rangle, \tag{3.24b}$$

where we have used the fact that $\hat{\mathbf{W}}$ and $\hat{\mathbf{G}}$ are nonrandom quantities. If we now require that the ensemble average of the transition operator be zero we conclude from Eqs. (3.24) that

$$\hat{\mathbf{W}} = \hat{\Gamma}^e - \hat{\Gamma}^0 = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle. \tag{3.25}$$

The operator $\hat{\Gamma}_e$ that determines the ensemble averaged Green dyadic $\hat{\mathbf{G}}$ is thus expressible in terms of the operator $\hat{\Gamma}^0$ and the ensemble average of the $\hat{\mathbf{Q}}^{(n)}$ operators. The actual calculation of this average is rather tedious and has, for this reason, been relegated to Appendix A. The result of the calculation using the quasicrystalline approximation (QCA) is that

$$\hat{\mathbf{W}} = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle = \bar{n} \int d^3R \hat{\mathbf{Q}}(\mathbf{R}), \tag{3.26}$$

where $\bar{n} = N/V$ is the number of scattering centers per unit volume and $\hat{\mathbf{Q}}(\mathbf{R})$ is the solution to the integral equation

$$\hat{\mathbf{Q}}(\mathbf{R}) = \hat{\mathbf{t}}(\mathbf{R}) + \hat{\mathbf{t}}(\mathbf{R}) \cdot \hat{\mathbf{G}} \cdot \int d^3R' \gamma(|\mathbf{R}' - \mathbf{R}|) \hat{\mathbf{Q}}(\mathbf{R}'). \tag{3.27}$$

In Eq. (3.27) $\gamma(|\mathbf{R}' - \mathbf{R}|)$ is the correlation function defined in Eq. (3.7) and $\mathbf{t}(\mathbf{R})$ is the average over all orientations of the transition operator describing single scattering from the elastic inhomogeneity $\delta C_{ijkl}^{(n)}, \delta\rho^{(n)}$ centered at the point $\mathbf{R}_n = \mathbf{R}$ in the medium characterized by the mean Green dyadic. $\hat{\mathbf{t}}(\mathbf{R})$ is thus given by

$$\hat{\mathbf{t}}(\mathbf{R}) = E[\hat{\mathbf{T}}(\mathbf{R})], \tag{3.28}$$

where $\hat{\mathbf{T}}(\mathbf{R})$ satisfies the operator equation

$$\hat{\mathbf{T}}(\mathbf{R}) = \delta\hat{\Gamma}^{(n)} + \delta\hat{\Gamma}^{(n)} \cdot \hat{\mathbf{G}} \cdot \hat{\mathbf{T}}(\mathbf{R}), \tag{3.29}$$

with $\delta\hat{\Gamma}^{(n)}$ being defined in Eq. (3.12a) for the case $\mathbf{R}_n = \mathbf{R}$. The notation $E[x]$ is the same as that used earlier and stands for the average of x over all orientations of the nth scatterer.

On substituting Eq. (3.26) into Eq. (3.25) we find that

$$\hat{\Gamma}^e = \hat{\Gamma}^0 + \bar{n} \int d^3R \hat{\mathbf{Q}}(\mathbf{R}), \tag{3.30}$$

so that Eq. (3.21) satisfied by the average Green dyadic becomes:

$$\left[\hat{\Gamma}^0 + \bar{n} \int d^3R \hat{\mathbf{Q}}(\mathbf{R})\right] \cdot \hat{\mathbf{G}} = -\hat{\mathbf{I}}. \tag{3.31}$$

The average Green dyadic is determined by simultaneously solving Eqs. (3.27) and (3.31) and the ensemble average of Eq. (3.29) over all orientations of the nth scatterer.

We conclude this Section by noting that the problem of determining the average Green dyadic $\langle \hat{\mathbf{g}} \rangle$ is equivalent to that of determining an "effective medium" which, as far as average propagation characteristics are concerned, is equivalent to the actual random medium. To see that this is so, imagine that the random medium is embedded in an infinite homogeneous and isotropic matrix characterized by the average Green dyadic $\langle \hat{\mathbf{g}} \rangle$. Consider now an elastic wave $|\psi\rangle$ propagating in the matrix and scattering off the sample of the random composite. The scattered field $|\psi^{(s)}\rangle$ is then given by

$$|\psi^{(s)}\rangle = \langle \hat{\mathbf{g}} \rangle \cdot \hat{\mathscr{T}} \cdot |\psi\rangle \tag{3.32}$$

so that the condition $\langle \hat{\mathscr{T}} \rangle = \mathbf{0}$ means that the average scattered field vanishes. This implies that, as far as the mean displacement field is concerned, the random medium is indistiguishable from the homogeneous, isotropic matrix in which it is embedded. This later observation then suggests that we identify this matrix as being the "effective medium" and take the parameters λ^e, μ^e, and ρ^e that characterize this matrix to be the effective Lamé constants and density of the random composite.

4. DISPERSION RELATIONS FOR THE EFFECTIVE MEDIUM

We ended the preceding section with the observation that the average Green dyadic characterizes a homogeneous, isotropic "effective" medium which, as far as average propagation characteristics are concerned, is equivalent to the random medium. We shall, in this section, derive dispersion relations satisfied by elastic plane-wave modes of the effective medium. These dispersion relations are important in that they determine the average propagation characteristics of the random medium. More specifically, the solutions to these dispersion relations yield the velocity and attenuation of coherent elastic waves propagating in the random medium and, in so doing, yield values for the effective Lamé constants λ^e, μ^e and effective density ρ^e.

The modes $|\psi\rangle$ of the effective medium are solutions to the equation

$$\hat{\Gamma}^e \cdot |\psi\rangle = \mathbf{0}. \tag{4.1}$$

Since $\hat{\Gamma}^e$ characterizes average wave propagation in the random medium Eq. (4.1) is satisfied by average elastic waves (coherent waves) propagating in this medium. On substituting for $\hat{\Gamma}^e$ from Eq. (2.17) we find that Eq. (4.1) can be expressed in the momentum representation as follows:

$$[(\lambda^e + 2\mu^e)\mathbf{pp} + \mu^e(p^2\mathbf{I} - \mathbf{pp}) - \omega^2\rho^e\mathbf{I}] \cdot \psi(\mathbf{p}) = 0. \tag{4.2}$$

In Eq. (4.2) $\psi(\mathbf{p}) = \langle \mathbf{p}|\psi\rangle$ is the mode $|\psi\rangle$ in the momentum representation and λ^e, μ^e, and ρ^e are the eigenvalues of $\hat{\lambda}^e$, $\hat{\mu}^e$, and $\hat{\rho}^e$ in this representation. These eigenvalues are the effective parameters of the random medium and may depend on the momentum vector $\mathbf{p}$.[42]

We now take the dot product of Eq. (4.2) with unit vectors $\hat{\mathbf{a}}_1$ and $\hat{\mathbf{a}}_2$ where $\hat{\mathbf{a}}_1$ is colinear with $\mathbf{p}$ and $\hat{\mathbf{a}}_2$ is perpendicular to $\mathbf{p}$. We obtain

$$[(\lambda^e + 2\mu^e)p^2 - \omega^2\rho^e]\hat{\mathbf{a}}_1 \cdot \psi(\mathbf{p}) = 0, \tag{4.3a}$$

$$[\mu^e p^2 - \omega^2\rho^e]\hat{\mathbf{a}}_2 \cdot \psi(\mathbf{p}) = 0. \tag{4.3b}$$

An examination of Eqs. (4.3) indicates that the amplitude $\psi(\mathbf{p})$ must either lie in the direction of $\mathbf{p}$, $(\hat{\mathbf{a}}_2 \cdot \psi(\mathbf{p}) = 0)$, or it must lie in the plane which is perpendicular to $\mathbf{p}$, $(\hat{\mathbf{a}}_1 \cdot \psi(\mathbf{p}) = 0)$. An elastic wave of the first type is called a

compressional wave and from Eq. (4.3a) has a wave number p_1 which must satisfy the dispersion relation

$$(\lambda^e + 2\mu^e)p_1^2 - \omega^2\rho^e = 0. \tag{4.4a}$$

An elastic wave of the second type is called a *shear* wave and has a wave number p_2 which must satisfy the dispersion relation

$$\mu^e p_2^2 - \omega^2\rho^e = 0. \tag{4.4b}$$

We can express the dispersion relations in terms of the properties of the random medium by substituting Eq. (3.30) for $\hat{\Gamma}^e$ into Eq. (4.1). We obtain

$$\left[\hat{\Gamma}^0 + \bar{n}\int d^3R\hat{\mathbf{Q}}(\mathbf{R})\right]\cdot|\psi\rangle = 0. \tag{4.5}$$

On making use of the operator identity[43]

$$\hat{\mathbf{Q}}(\mathbf{R}) \equiv e^{-i\hat{\mathbf{p}}\cdot\mathbf{R}}\hat{\mathbf{Q}}(\mathbf{R}=\mathbf{0})e^{i\hat{\mathbf{p}}\cdot\mathbf{R}} \tag{4.6}$$

we find that in the momentum representation Eq. (4.5) becomes

$$[(\lambda^0 + 2\mu^0)\mathbf{pp} + \mu^0(p^2\mathbf{I} - \mathbf{pp}) - \omega^2\rho^0\mathbf{I} + (2\pi)^3\bar{n}\mathbf{Q}(\mathbf{p},\mathbf{p})]\cdot\psi(\mathbf{p}) = 0, \tag{4.7}$$

where

$$\mathbf{Q}(\mathbf{p},\mathbf{p}) = \langle\mathbf{p}|\hat{\mathbf{Q}}(\mathbf{R}=\mathbf{0})|\mathbf{p}\rangle \tag{4.8}$$

is the diagonal matrix element of $\hat{\mathbf{Q}}(\mathbf{R}=\mathbf{0})$ in the momentum representation.

The dispersion relation for the compressional mode is obtained by taking the dot product of Eq. (4.7) with $\hat{\mathbf{a}}_1$ and making use of the fact that for compression waves $\psi(\mathbf{p})$ and $\mathbf{p}$ are colinear with $\hat{\mathbf{a}}_1$. We then find that

$$(\lambda^0 + 2\mu^0)p_1^2 - \omega^2\rho^0 + (2\pi)^3\bar{n}\hat{\mathbf{a}}_1\cdot\mathbf{Q}(\mathbf{p}_1,\mathbf{p}_1)\cdot\hat{\mathbf{a}}_1 = 0. \tag{4.9a}$$

In a similar fashion we find upon taking the dot product of Eq. (4.7) with $\hat{\mathbf{a}}_2$ that the dispersion relation for the shear wave mode is given by

$$\mu^0 p_2^2 - \omega^2\rho^0 + (2\pi)^3\bar{n}\hat{\mathbf{a}}_2\cdot\mathbf{Q}(\mathbf{p}_2,\mathbf{p}_2)\cdot\hat{\mathbf{a}}_2 = 0. \tag{4.9b}$$

The matrix elements $\mathbf{Q}(\mathbf{p},\mathbf{p}')$ obey an integral equation which is obtained by taking the matrix elements of Eq. (3.27) in the momentum representation and making use of the operator identity given in Eq. (4.6). One finds that

$$\mathbf{Q}(\mathbf{p},\mathbf{p}') = \mathbf{t}(\mathbf{p},\mathbf{p}') + \int d^3p''\mathbf{t}(\mathbf{p},\mathbf{p}'')\cdot\mathbf{G}(\mathbf{p}'')\cdot\mathbf{Q}(\mathbf{p}'',\mathbf{p}')\tilde{\gamma}(\mathbf{p}''-\mathbf{p}'), \tag{4.10}$$

where

$$\mathbf{t}(\mathbf{p},\mathbf{p}') = \langle\mathbf{p}|\hat{\mathbf{t}}(\mathbf{R}=\mathbf{0})|\mathbf{p}'\rangle, \tag{4.11a}$$

$$\mathbf{G}(\mathbf{p}'')\delta(\mathbf{p}-\mathbf{p}'') = \langle\mathbf{p}|\hat{\mathbf{G}}|\mathbf{p}''\rangle, \tag{4.11b}$$

and

$$\tilde{\gamma}(\mathbf{K}) = \int d^3R\,\gamma(|\mathbf{R}|)e^{-i\mathbf{K}\cdot\mathbf{R}}. \tag{4.12}$$

We shall consider here only the limiting case of a completely random distribution of scatterers for which the correlation function $\gamma(|\mathbf{R}|)$ vanishes. In this case $\mathbf{Q}(\mathbf{p},\mathbf{p}) = \mathbf{t}(\mathbf{p},\mathbf{p})$ and the dispersion relations (4.9a) and (4.9b) become

$$(\lambda^0 + 2\mu^0)p_1^2 - \omega^2\rho^0 + (2\pi)^3\bar{n}E[\hat{\mathbf{a}}_1\cdot\mathbf{T}(\mathbf{p}_1,\mathbf{p}_1)\cdot\hat{\mathbf{a}}_1] = 0, \tag{4.13a}$$

$$\mu^0 p_2^2 - \omega^2\rho^0 + (2\pi)^3\bar{n}E[\hat{\mathbf{a}}_2\cdot\mathbf{T}(\mathbf{p}_2,\mathbf{p}_2)\cdot\hat{\mathbf{a}}_2] = 0. \tag{4.13b}$$

In deriving Eqs. (4.13) we have made use of Eq. (3.28) and have defined

$$\mathbf{T}(\mathbf{p},\mathbf{p}) = \langle\mathbf{p}|\hat{\mathbf{T}}(\mathbf{R}=\mathbf{0})|\mathbf{p}\rangle. \tag{4.14}$$

The quantities $\hat{\mathbf{a}}_j\cdot\mathbf{T}(\mathbf{p}_j,\mathbf{p}_j)\cdot\hat{\mathbf{a}}_j$ are intimately related to the compressional and shear wave scattering amplitudes produced by the elastic inhomogeneity $\delta C^{(n)}_{ijkl}$, $\delta\rho^{(n)}$ centered at the origin $\mathbf{R}_n = \mathbf{0}$ in the effective medium. In particular, it is shown in Appendix B that

$$\hat{\mathbf{a}}_j\cdot\mathbf{T}(\mathbf{p}_j,\mathbf{p}_j)\cdot\hat{\mathbf{a}}_j = -\frac{\rho^e\omega^2}{2\pi^2 p_j^2}\hat{\mathbf{a}}_j\cdot\mathbf{A}_j(\mathbf{p}_j,\mathbf{p}_j), \tag{4.15}$$

where $\mathbf{A}_1(\mathbf{p}_1,\mathbf{p}_1)$ is the compressional wave scattering amplitude in the forward direction produced by a compressional plane wave mode $\hat{\mathbf{a}}_1|\mathbf{p}_1\rangle$ incident to the inhomogeneity $\delta C^{(n)}_{ijkl}$, $\delta\rho^{(n)}$ centered at the origin in the effective medium. Similarly, $\mathbf{A}_2(\mathbf{p}_2,\mathbf{p}_2)$ is the shear wave scattering amplitude in the forward direction produced by a shear plane wave mode $\hat{\mathbf{a}}_2|\mathbf{p}_2\rangle$ incident to this inhomogeneity embedded in the effective medium. On substituting Eq. (4.15) into (4.13) we find that the dispersion relations assume the forms

$$(\lambda^0 + 2\mu^0)p_1^2 - \omega^2\rho^0 - 4\pi\frac{\rho^e\omega^2}{p_1^2}\bar{n} \times E[\hat{\mathbf{a}}_1\cdot\mathbf{A}_1(\mathbf{p}_1,\mathbf{p}_1)] = 0, \tag{4.16a}$$

$$\mu^0 p_2^2 - \omega^2\rho^0 - 4\pi\frac{\rho^e\omega^2}{p_2^2}\bar{n}E[\hat{\mathbf{a}}_2\cdot\mathbf{A}_2(\mathbf{p}_2,\mathbf{p}_2)] = 0. \tag{4.16b}$$

Equations (4.16) are of practical importance since the forward scattering amplitudes $\mathbf{A}_j(\mathbf{p}_j,\mathbf{p}_j)$ can be approximately calculated for homogeneous, isotropic scatterers of various shapes. To illustrate the usefulness of these relations we shall apply them to calculate the effective Lamé constants and density of a completely random distribution of homogeneous, isotropic inclusions whose Lamé constants λ,μ and density ρ differ only slightly from those of the matrix; i.e., from λ^0, μ^0 and ρ^0. For this case we can use the Born approximations to the forward scattering amplitudes $\mathbf{A}_j(\mathbf{p}_j,\mathbf{p}_j)$. These quantities were calculated for arbitrary inclusion shapes by Gubernatis *et al.*[21] and we find that

$$\hat{\mathbf{a}}_1\cdot\mathbf{A}_1(\mathbf{p}_1,\mathbf{p}_1) = \frac{p_1^2}{4\pi}\left[\frac{\delta\rho}{\rho^e} - \frac{\delta\lambda + 2\delta\mu}{\lambda^e + 2\mu^e}\right]v, \tag{4.17a}$$

$$\hat{\mathbf{a}}_2\cdot\mathbf{A}_2(\mathbf{p}_2,\mathbf{p}_2) = \frac{p_2^2}{4\pi}\left[\frac{\delta\rho}{\rho^e} - \frac{\delta\mu}{\mu^e}\right]v. \tag{4.17b}$$

In Eqs. (4.17) v is the volume of an inclusion and $\delta\lambda = \lambda - \lambda^0$, $\delta\mu = u - \mu^0$ and $\delta\rho = \rho - \rho^0$.

On substituting Eqs. (4.17) into (4.16) we find that

$$[(\lambda^0 + 2\mu^0) + \mathbf{C}(\delta\lambda + 2\delta\mu)]p_1^2 - \omega^2[\rho^0 + C\delta\rho] = 0, \tag{4.18a}$$

$$[\mu^0 + \mathbf{C}\delta\mu]p_2^2 - \omega^2[\rho^0 + C\delta\rho] = 0, \tag{4.18b}$$

where $C = \bar{n}v$ is the volume concentration of inclusions and where we have made use of Eqs. (4.4). On comparing Eqs. (4.18) with Eqs. (4.4) we conclude that the effective Lamé constants and density are given by

$$\lambda^e = \lambda^0 + C\delta\lambda, \tag{4.19a}$$

$$\mu^e = \mu^0 + C\delta\mu, \tag{4.19b}$$

$$\rho^e = \rho^0 + C\delta\rho. \tag{4.19c}$$

The parameters λ^e, μ^e and ρ^e characterizing the average medium are thus found to be the volume weighted average of the Lamé constants and density of the two phases comprising the random medium. This result is the lowest order approximation of the theory developed in this paper (Born approximation in the CPA) and is known to be a limiting bound on the effective material parameters.[44] It is interesting to note that in this lowest order approximation the effective material parameters are *real* and independent of the momentum vector $\mathbf{p}$. The fact that these parameters are real is a consequences of our using the Born approximation for the forward scattering amplitudes and implies that the effective medium is nonabsorbing and nonspatially dispersive. When the differences $\delta\lambda$, $\delta\mu$ and $\delta\rho$ between the inclusion and matrix parameters becomes large the coherent elastic waves will attenuate due to scattering losses. In this case one cannot employ the Born approximation and one would find that the forward scattering amplitudes $\mathbf{A}_j(\mathbf{p}_j,\mathbf{p}_j)$ will become complex. The effective Lamé constants λ^e and μ^e will then be complex so that the effective medium will be absorbing.

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APPENDIX A: CALCULATION OF $\hat{\mathbf{W}} = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle$

In this appendix we employ the so-called *quasicrystalline approximation* (QCA) to calculate the average of the operator $\Sigma_{n=1}^{N} \hat{\mathbf{Q}}^{(n)}$ over the ensemble of scatterer locations and orientations. Strictly speaking, the QCA applies only to the calculation of averages over scatterer locations so that in the treatment presented below we have had to generalize this concept so as to apply also to our calculation of an average over the ensemble of scatterer orientations. This generalization appears justifiable in that it is a natural extension of the QCA technique and will reduce to the usual QCA in the case that all scatterers have identical orientations.

The $\hat{\mathbf{Q}}^{(n)}$ operator is defined in Eqs. (3.22) and (3.23a). If we substitute Eq. (3.22) into (3.23a) we find that $\hat{\mathbf{Q}}^{(n)}$ satisfies the equation

$$[\hat{\mathbf{I}} - \delta\hat{\mathbf{\Gamma}}^{(n)}\cdot\hat{\mathbf{G}}]\cdot\hat{\mathbf{Q}}^{(n)} = \delta\hat{\mathbf{\Gamma}}^{(n)} + \delta\hat{\mathbf{\Gamma}}^{(n)}\cdot\left[\sum_{n'\neq n}\hat{\mathbf{Q}}^{(n')} - \hat{\mathbf{q}}\right], \tag{A1}$$

where the notation $n' \neq n$ means to sum over all values of n' not equal to n and $\hat{\mathbf{I}}$ is the identity dyadic operator. We now define the *single scattering transition operator* characterizing scattering by the scatterer $\delta\hat{\mathbf{\Gamma}}^{(n)}$ embedded in the average medium. This operator obeys the equation

$$\hat{\mathbf{t}}^{(n)} = \delta\hat{\mathbf{\Gamma}}^{(n)} + \delta\hat{\mathbf{\Gamma}}^{(n)}\cdot\hat{\mathbf{G}}\cdot\hat{\mathbf{t}}^{(n)}. \tag{A2}$$

On rearranging Eq. (A2) we obtain

$$\delta\hat{\mathbf{\Gamma}}^{(n)} = [\hat{\mathbf{I}} - \delta\hat{\mathbf{\Gamma}}^{(n)}\cdot\hat{\mathbf{G}}]\cdot\hat{\mathbf{t}}^{(n)}, \tag{A3}$$

which when substituted into the right-hand side of Eq. (A1) gives the result that

$$\hat{\mathbf{Q}}^{(n)} = \hat{\mathbf{t}}^{(n)} + \hat{\mathbf{t}}^{(n)}\cdot\hat{\mathbf{G}}\cdot\left[\sum_{n'\neq n}\hat{\mathbf{Q}}^{(n')} - \hat{\mathbf{q}}\right]. \tag{A4}$$

We require the ensemble average of $\hat{\mathbf{Q}}^{(n)}$ defined in Eq. (A4) over all orientations and locations of the N scatterers. We shall first perform the average over the orientations of the scatterers for a fixed realization of their locations. If we fix the orientation of the nth scatterer we find from Eq. (A4) that

$$E_n[\hat{\mathbf{Q}}^{(n)}] = \hat{\mathbf{t}}^{(n)} + \hat{\mathbf{t}}^{(n)}\cdot\hat{\mathbf{G}}\cdot\left\{\sum_{n'\neq n}E_n[\hat{\mathbf{Q}}^{(n')}] - E_n[\hat{\mathbf{q}}]\right\}, \tag{A5}$$

where the notation $E_n[x]$ stands for the average of x over the ensemble of orientations of all scatterers *other* than the n'th (i.e., with the orientation of the n'th scatterer held fixed).

We now assume that the conditional averages $E_n[\hat{\mathbf{Q}}^{(n')}]$ and $E_n[\hat{\mathbf{q}}]$ appearing on the right-hand side of Eq. (A5) can be replaced by the unconditional averages (i.e., the averages over the ensemble of *all* scatterer orientations) $E[\hat{\mathbf{Q}}^{(n')}]$ and $E[\hat{\mathbf{q}}]$. Because of the assumed statistical independence of the orientation of different scatterers this assumption amounts to applying the QCA to the distribution of scatterer orientations. On making this approximation in Eq. (A5) and then averaging the resulting equation over the orientation of the n'th scatterer we obtain

$$E[\hat{\mathbf{Q}}^{(n)}] = \hat{\mathbf{t}}_n + \hat{\mathbf{t}}_n\cdot\hat{\mathbf{G}}\cdot\left[\sum_{n'\neq n}E[\hat{\mathbf{Q}}^{(n')}] - E[\hat{\mathbf{q}}]\right], \tag{A6}$$

where $\hat{\mathbf{t}}_n$ is the average of $\hat{\mathbf{t}}^{(n)}$ over the orientation of the n'th scatterer. The quantities $E[\hat{\mathbf{Q}}^{(n)}]$ and $E[\hat{\mathbf{q}}]$ depend on the ensemble of scatterer locations $\{\mathbf{R}_1,...,\mathbf{R}_N\}$ while $\hat{\mathbf{t}}_n$ depends only on the location of the n'th scatterer.

We shall now apply the QCA to the calculation of the average of $E[\hat{\mathbf{Q}}^{(n)}]$ over the ensemble of scattering centers. To this end we define the quantities

$$\hat{\mathbf{Q}}(\mathbf{R}_n) = \int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,...,\mathbf{R}_N|\mathbf{R}_n) \times E[\hat{\mathbf{Q}}^{(n)}], \tag{A7a}$$

$$\hat{\mathbf{Q}}(\mathbf{R}_n,\mathbf{R}_{n'}) = \int d^3R_1 \cdots dR_N P(\mathbf{R}_1,...,\mathbf{R}_N|\mathbf{R}_n,\mathbf{R}_{n'}) \times E[\hat{\mathbf{Q}}^{(n)}], \tag{A7b}$$

where $P(\mathbf{R}_1,...,\mathbf{R}_N|\mathbf{R}_n)$ is the conditional probability density function for the configuration $\{\mathbf{R}_1,...,\mathbf{R}_N\}$ given that $\mathbf{R}_n$ is held fixed, and $P(\mathbf{R}_1,...,\mathbf{R}_N|\mathbf{R}_n,\mathbf{R}_{n'})$ is the conditional density function when both $\mathbf{R}_{n'}$ and $\mathbf{R}_n$, are held fixed. The notation $d^3R_1 \cdots d^3R_N$ means to integrate over all scatterer locations except $\mathbf{R}_n$ and $d^3R_1 \cdots d^3R_N$ means to integrate over all locations except $\mathbf{R}_n$ and $\mathbf{R}_{n'}$. We note that the total ensemble average of $\hat{\mathbf{Q}}^{(n)}$ is

$$\langle \hat{\mathbf{Q}}^{(n)} \rangle = \int d^3R_n P(\mathbf{R}_n)\hat{\mathbf{Q}}(\mathbf{R}_n). \tag{A8}$$

On substituting $E[\hat{\mathbf{Q}}^{(n)}]$ from Eq. (A6) into Eq. (A7a) we obtain

$$\hat{\mathbf{Q}}(\mathbf{R}_n) = \hat{\mathbf{t}}_n + \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \sum_{n' \neq n} \int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) \times E[\hat{\mathbf{Q}}^{(n')}] - \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \int d^3R_1 \cdots d^3R_N \times P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) E[\hat{\mathbf{q}}]. \tag{A9}$$

Now, we can put

$$P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) = P(\mathbf{R}_{n'}|\mathbf{R}_n) P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n,\mathbf{R}_{n'}) \tag{A10}$$

to find that

$$\int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) E[\hat{\mathbf{Q}}^{(n')}] = \int d^3\mathbf{R}_{n'} P(\mathbf{R}_{n'}|\mathbf{R}_n) \hat{\mathbf{Q}}(\mathbf{R}_n,\mathbf{R}_{n'}), \tag{A11}$$

where we have made use of Eq. (A7b) and where $P(\mathbf{R}_{n'}|\mathbf{R}_n)$ is the conditional probability density function for $\mathbf{R}_{n'}$ given that $\mathbf{R}_n$ is fixed. On substituting Eq. (A11) into Eq. (A9) we obtain

$$\hat{\mathbf{Q}}(\mathbf{R}_n) = \hat{\mathbf{t}}_n + \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \sum_{n' \neq n} \int d^3R_{n'} P(\mathbf{R}_{n'}|\mathbf{R}_n) \hat{\mathbf{Q}}(\mathbf{R}_n,\mathbf{R}_{n'}) - \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) E[\hat{\mathbf{q}}]. \tag{A12}$$

The QCA consists of making the approximations:

$$\hat{\mathbf{Q}}(\mathbf{R}_n,\mathbf{R}_{n'}) \approx \hat{\mathbf{Q}}(\mathbf{R}_{n'}), \tag{A13a}$$

$$\int d^3R_1 \cdots d^3R_N P(\mathbf{R}_1,\ldots,\mathbf{R}_N|\mathbf{R}_n) \mathbf{E}[\hat{\mathbf{q}}] \approx \langle \hat{\mathbf{q}} \rangle. \tag{A13b}$$

If we apply the QCA to Eq. (A12) we obtain

$$\hat{\mathbf{Q}}(\mathbf{R}_n) = \hat{\mathbf{t}}_n + \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \sum_{n' \neq n} \int d^3R_{n'} P(\mathbf{R}_{n'}|\mathbf{R}_n) \hat{\mathbf{Q}}(\mathbf{R}_{n'}) - \hat{\mathbf{t}}_n \cdot \hat{\mathbf{G}} \cdot \langle \hat{\mathbf{q}} \rangle. \tag{A14}$$

Since the scatterer locations are assumed to be identically distributed, we have that

$$\int d^3R_{n'} P(\mathbf{R}_{n'}|\mathbf{R}_n) \hat{\mathbf{Q}}(\mathbf{R}_{n'}) = \int d^3\mathbf{R}' P(\mathbf{R}'|\mathbf{R}) \hat{\mathbf{Q}}(\mathbf{R}'), \tag{A15}$$

independent of n and n' and

$$\langle \hat{\mathbf{q}} \rangle = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle = N \int d^3R' P(\mathbf{R}') \hat{\mathbf{Q}}(\mathbf{R}'), \tag{A16}$$

where we have made use of Eq. (A8)

On making use of Eqs. (A15) and (A16) in Eq. (A14) we find that

$$\hat{\mathbf{Q}}(\mathbf{R}) = \hat{\mathbf{t}}(\mathbf{R}) + \hat{\mathbf{t}}(\mathbf{R}) \cdot \hat{\mathbf{G}} \cdot \int d^3R' \gamma(|\mathbf{R} - \mathbf{R}'|) \hat{\mathbf{Q}}(\mathbf{R}'), \tag{A17}$$

where

$$\gamma(|\mathbf{R} - \mathbf{R}'|) = (N-1) P(\mathbf{R}'|\mathbf{R}) - NP(\mathbf{R}'), \tag{A18}$$

and where $\hat{\mathbf{t}}(\mathbf{R})$ is the single scattering transition operator for the scatterer centered at the point $\mathbf{R}$ averaged over all orientations of the scatterer. The $\hat{\mathbf{W}}$ operator defined in Eq. (3.12b) is thus given by

$$\hat{\mathbf{W}} = \sum_{n=1}^{N} \langle \hat{\mathbf{Q}}^{(n)} \rangle = N \int d^3R P(\mathbf{R}) \hat{\mathbf{Q}}(\mathbf{R}) = \bar{n} \int d^3R \hat{\mathbf{Q}}(\mathbf{R}), \tag{A19}$$

with $\hat{\mathbf{Q}}(\mathbf{R})$ being the solution of the integral equation (A17) and where

$$\bar{n} = NP(\mathbf{R}) = N/V \tag{A20}$$

is the average number of scatterers per unit volume.

APPENDIX B: DERIVATION OF EQ. (4.15)

We wish to relate the quantities $\hat{\mathbf{a}}_j \cdot \mathbf{T}(\mathbf{p}_j,\mathbf{p}_j) \cdot \hat{\mathbf{a}}_j$ appearing in the dispersion relations (4.13) to the forward scattering amplitudes $\mathbf{A}_j(\mathbf{p}_j,\mathbf{p}_j)$ according to Eq. (4.15). Toward this end we consider the elastic inhomogeneity $\delta C^{(n)}_{ijkl}$, $\delta\rho^{(n)}$ centered at the origin ($\mathbf{R}_n = \mathbf{0}$) in the effective medium. The field scattered by this inhomogeneity is equal to

$$|\psi^{(s)}\rangle = \hat{\mathbf{G}} \cdot \hat{\mathbf{T}}(\mathbf{R} = \mathbf{0}) \cdot |\psi^{(i)}\rangle, \tag{B1}$$

where $|\psi^{(i)}\rangle$ is the incident field, $\hat{\mathbf{G}} = \langle \hat{\mathbf{g}} \rangle$ the average Green tensor characterizing the effective medium and $\hat{\mathbf{T}}(\mathbf{R} = \mathbf{0})$ the transition operator whose matrix elements in the momentum representation are given by Eq. (4.14).

Choosing $|\psi^{(i)}\rangle$ to be a plane-wave $\hat{\mathbf{a}}_j|\mathbf{p}_j\rangle$ and evaluating Eq. (B1) in the coordinate representation yields

$$\psi^{(s)}(\mathbf{r}) = \langle \mathbf{r}|\psi^{(s)}\rangle = \int d^3p' \int d^3r' \hat{\mathbf{G}}(\mathbf{r} - \mathbf{r}') \cdot \mathbf{T}(\mathbf{p}',\mathbf{p}_j) \cdot \hat{\mathbf{a}}_j e^{i\mathbf{p}' \cdot \mathbf{r}'}, \tag{B2}$$

where $\hat{\mathbf{G}}(\mathbf{r} - \mathbf{r}') = \langle \mathbf{r}|\hat{\mathbf{G}}|\mathbf{r}'\rangle$ is the matrix element of $\hat{\mathbf{G}}$ in the coordinate representation. This quantity is readily obtained by solving Eq. (3.21) in the coordinate representation and is found to be[45]

$$\hat{\mathbf{G}}(\mathbf{r} - \mathbf{r}') = \frac{-1}{4\pi\rho^e\omega^2} \left[p_2^2 \frac{e^{ip_2|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \mathbf{I} - \nabla\nabla \times \left(\frac{e^{ip_1|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} - \frac{e^{ip_2|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \right) \right]. \tag{B3}$$

We wish to evaluate Eq. (B2) in the far field (i.e., as $p_1 r \to \infty$ and $p_2 r \to \infty$). In this limit Eq. (B3) gives

$$\hat{\mathbf{G}}(\mathbf{r} - \mathbf{r}') \sim \frac{-1}{4\pi\rho^e\omega^2} \left[p_2^2 (\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}) e^{-ip_2 \hat{\mathbf{r}} \cdot \hat{\mathbf{r}}'} \frac{e^{ip_2 r}}{r} + p_1^2 \hat{\mathbf{r}}\hat{\mathbf{r}} e^{-ip_1 \hat{\mathbf{r}} \cdot \mathbf{r}'} \frac{e^{ip_1 r}}{r} \right], \tag{B4}$$

where $\hat{\mathbf{r}} = \mathbf{r}/r$ is the unit vector in the $\mathbf{r}$ direction. On substituting Eq. (B4) into Eq. (B2) we obtain

$$\psi^{(s)}(\mathbf{r}) \sim \mathbf{A}_1(p_1\hat{\mathbf{r}},\mathbf{p}_j) \frac{e^{ip_1 r}}{r} + \mathbf{A}_2(p_2\hat{\mathbf{r}},\mathbf{p}_j) \frac{e^{ip_2 r}}{r}, \tag{B5}$$

where

$$\mathbf{A}_1(p_1\hat{\mathbf{r}},\mathbf{p}_j) = \frac{-2\pi^2 p_1^2}{\rho^e\omega^2} \hat{\mathbf{r}}\hat{\mathbf{r}} \cdot \mathbf{T}(p_1\hat{\mathbf{r}},\mathbf{p}_j) \cdot \hat{\mathbf{a}}_j, \tag{B6a}$$

$$\mathbf{A}_2(p_2\hat{\mathbf{r}},\mathbf{p}_j) = \frac{-2\pi^2 p_2^2}{\rho^e\omega^2} (\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}) \cdot \mathbf{T}(p_2\hat{\mathbf{r}},\mathbf{p}_j) \cdot \hat{\mathbf{a}}_j. \tag{B6b}$$

The quantities $\mathbf{A}_1(p_1\hat{\mathbf{r}},\mathbf{p}_j)$ and $\mathbf{A}_2(p_2\hat{\mathbf{r}},\mathbf{p}_j)$ are, respectively, the compressional and shear wave scattering amplitudes produced by the incident plane wave $\hat{\mathbf{a}}_j|\mathbf{p}_j\rangle$. Evaluating Eqs. (B6) in the *forward direction* (i.e., when $\hat{\mathbf{r}} = \hat{\mathbf{p}}_j = \mathbf{p}_j/p_j$) and using the fact that $\hat{\mathbf{a}}_1 \cdot \hat{\mathbf{p}}_j = 1$ and

$\hat{\mathbf{a}}_2 \cdot \hat{\mathbf{p}}_j = 0$ then yields the required expressions given in Eqs. (4.15).

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[38]A somewhat similar integral equation has been derived by J. E. Gubernatis, E. Domany and J. A. Krumhansl [J. Appl. Phys. **48**, 2804 (1977)] for the scattering of an incident elastic wave from an inhomogeneity of arbitrary shape but constant material properties embedded in a homogeneous, isotropic matrix medium.
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[40]We shall denote operators by placing a carat "$\wedge$" over the symbol representing the associated physical quantity.
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[42]In order to satisfy the requirement $\langle \hat{\mathcal{F}} \rangle = \mathbf{0}$ the operators $\hat{\lambda}^c$, $\hat{\mu}^c$ and $\hat{\rho}^c$ will, in general, depend on the momentum operator $\hat{\mathbf{p}}$. As discussed in the introduction this means that the "average medium" is *spatially dispersive* and may possess more than one longitudinal and one transverse velocity.
[43]See, for example, P. Roman quoted in Ref. 17, Sec. 5.3.
[44]See, for example, Refs. 27 and 28.
[45]See, for example, the paper by J. E. Gubernatis et al. cited in Ref. 38. In that paper their Green tensor differs from ours by a factor of minus one which accounts for the sign difference between Eq. (B3) and their result [Eq. (2.27) in their paper.].

Lateral boundary conditions for quasisteady atmospheric flows

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The quasisteady model, derived by the author in an earlier paper, is extended to include lateral boundary conditions. The approach is to first specify a complete time-dependent problem, including boundary conditions; it is stressed that to each boundary condition there should be associated a precise physical assumption. Assuming the time-dependent problem is well-posed, it is then shown that the quasisteady assumption can be applied consistently to both the partial differential equations and the boundary conditions, thereby obtaining a well-posed mathematical model with time scales suitable for large scale atmospheric flows. Three types of conditions are considered at the lateral boundaries: (1) outflow, (2) inflow (driven)—velocity is specified and is essentially independent of the internal flow, (3) inflow (passive)—inflow is created primarily by the internal flow configuration. The upper boundary conditions include the two derived by the author in the earlier paper, the continuous and discontinuous boundary conditions, and a third condition, which is designed to allow the flow to propagate independently of the height of the region. Numerical solutions are obtained for various test cases, and convergence of the calculations is demonstrated. One sees that the calculations are reasonable, both from a mathematical and physical standpoint.

I. INTRODUCTION

Difficulties at free boundaries arise in almost all areas of fluid dynamics, although in the case of supersonic flow, the problems are generally simpler.[1] In many cases the model may be well-posed mathematically, but it is perhaps impossible to specify physically accurate boundary conditions. In the atmospheric problem, the equations may not even be well-posed.[2] This situation has led to a wide variety of numerical procedures. Some, by considering "computational boundary conditions", ignore both the mathematics and physics.[3,4] Some insist on the necessity of mathematically neither over-specifying nor under-specifying the number of boundary conditions.[5,6,7] In regard to the physics, at least in atmospheric problems, the general rule seems to be that physical interpretation of boundary conditions is not required.[8,9,10] In Ref. 11 quasisteady equations were derived on the basis of scale assumptions approximately satisfied in large-scale atmospheric flow. The purpose of the present paper is to extend this analysis to include inflow and outflow at the lateral boundaries. The derivation will attempt to proceed in two steps. First, boundary conditions will be specified for the time-dependent equations (Sec. II). The underlying principle here is that each boundary condition, since it must make an assumption regarding the external flow, must have a clearly defined physical interpretation. Assuming the time-dependent equations are well-posed,[12] the second step is to derive quasisteady equations by using the scale assumptions (Sec. III).

Calculations using the quasisteady model are described in Secs. IV, V, and VI: Sec. IV considers a problem involving internally generated flow, Section V considers a bell-shaped wave entering at a lateral boundary, and Sec. VI considers a "flat" wave entering at a lateral boundary. Section VII summarizes possible conclusions of the study. An accuracy study, in terms of a decreased mesh size, was conducted for all calculations. Results of this study are shown for the bell-wave calculation in Sec. V.

II. SPECIFICATION OF BOUNDARY CONDITIONS FOR THE COMPLETE TIME-DEPENDENT PROBLEM

The variables to be used are similar to those defined in Ref. 11, except that the velocity components are now normalized:

$$\tilde{u} = (u - aw)/(1 + a^2)^{1/2}, \tag{1.1}$$

$$\tilde{w} = (w + au)/(1 + a^2)^{1/2}, \tag{1.2}$$

$$\pi = \bar{p}^{(\gamma-1)/\gamma}, \tag{1.3}$$

$$\theta = (1/\bar{\rho})\,\bar{p}^{1/\gamma}. \tag{1.4}$$

Using the transformation

$$\tau = t, \tag{2.1}$$

$$\eta = x/L, \tag{2.2}$$

$$\zeta = \frac{z - f_1(t,x)}{f_2(t,x) - f_1(t,x)}, \tag{2.3}$$

The hydrodynamic equations, to be solved in the region $\{\tau > 0,\ 0 \leqslant \eta \leqslant 1,\ 0 \leqslant \zeta \leqslant 1\}$, take the following form:

$$\theta_\tau = -r\theta_\zeta - (u/L)\theta_\eta, \tag{3.1}$$

$$\begin{aligned}\tilde{u}_\tau = -G_1 = {} & -r\tilde{u}_\zeta - \frac{u}{L}\tilde{u}_\eta - \frac{c_s^2}{(\gamma-1)\pi L(1+a^2)^{1/2}}\pi_\eta \\ & + \frac{ag}{(1+a^2)^{1/2}} - \frac{\tilde{\omega}}{1+a^2}\left(a_\tau + ra_\zeta + \frac{u}{L}a_\eta\right),\end{aligned} \tag{3.2}$$

$$\begin{aligned}\pi_\tau = -G_2 = {} & -r\pi_\zeta - \frac{u}{L}\pi_\eta - \frac{(\gamma-1)\pi}{L(1+a^2)^{1/2}} \\ & \times(\tilde{u}_\eta + a\tilde{\omega}_\eta) - (\gamma-1)\pi\zeta_z(1+a^2)^{1/2}\tilde{\omega}_\zeta - \frac{(\gamma-1)\pi}{(1+a^2)^{1/2}} \\ & \times\left(\frac{w}{L(1+a^2)^{1/2}}a_\eta - \tilde{u}\zeta_z a_\zeta\right),\end{aligned} \tag{3.3}$$

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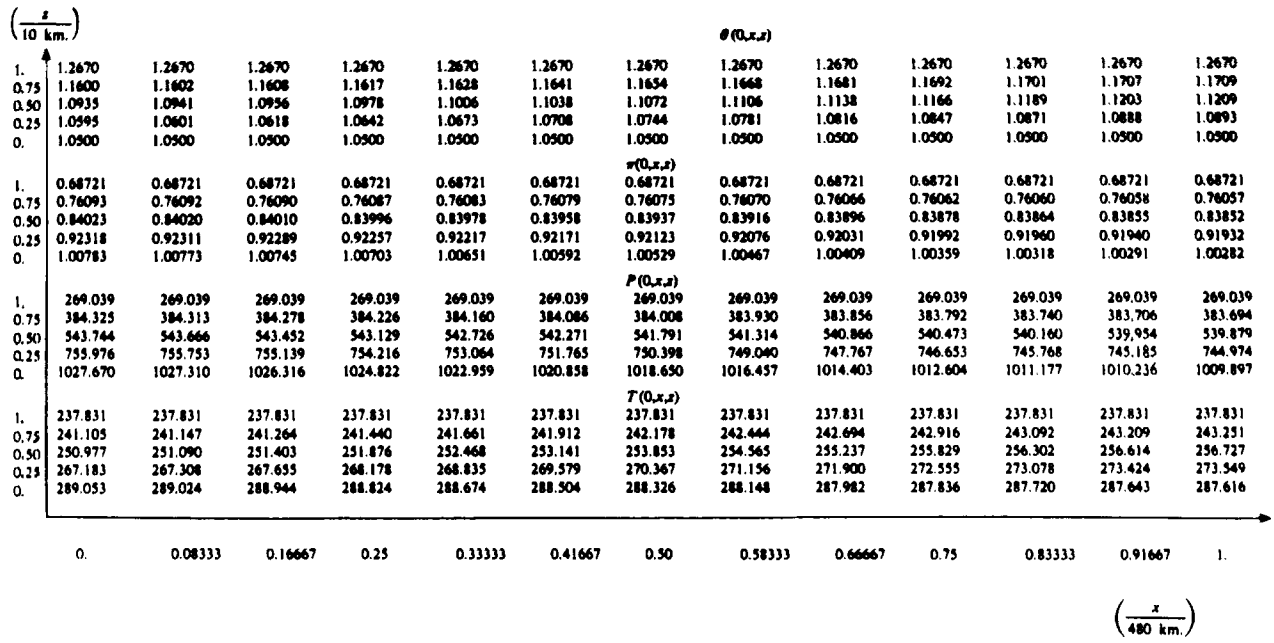

FIG. 1. Initial flow field.

$$\tilde{w}_\tau = -G_3 = -r\tilde{w}_\zeta - \frac{u}{L}\tilde{w} - \frac{c_s^2\zeta_z(1+a^2)^{1/2}}{(\gamma-1)\pi}\pi_\zeta - \frac{g}{(1+a^2)^{1/2}} - \frac{ac_s^2}{(\gamma-1)L(1+a^2)^{1/2}}\pi_\eta + \frac{\tilde{u}}{1+a^2}\left(a_\tau + ra_\zeta + \frac{u}{L}a_\eta\right). \tag{3.4}$$

The various parameters defined above are as follows:

$a = \zeta_x/\zeta_z, r = \zeta_t + w\zeta_z + u\zeta_x, \gamma = 1 + R/c_v, c_s^2 = \gamma RT,$

$\bar{P} = p/P_0, \bar{T} = T/T_0$, f_1 = position of the lower boundary, f_2 = position of upper boundary, ρ = density, T = temperature, w = vertical velocity, u = horizontal velocity, R = gas constant, c_v = specific heat, x = horizontal distance, z = vertical distance, t = time, g = acceleration due to gravity, p = pressure = ρRT, ρ_0 and T_0 are reference values.

The equations for the floating top and for the continuous and discontinuous boundary conditions [Ref. 11: Eqs. (10), (15), and (21)] take respectively the following forms:

$$(f_2)_\tau = \tilde{w}(1+a^2)^{1/2}, \tag{4.1}$$

$$\pi_\tau = \frac{(\gamma-1)\pi}{c_s}\tilde{w}_\tau, \tag{4.2}$$

$$\pi_\tau = \begin{cases} \dfrac{(\gamma-1)\pi}{c_s}\tilde{w}_\tau: & \tilde{w} \leqslant 0 \\ \dfrac{(\gamma-1)\pi}{c_s}\tilde{w}_\tau - \dfrac{(\gamma-1)\pi g}{c_s^2}(f_2)_\tau: & \tilde{w} > 0 \end{cases} \tag{4.3}$$

Remark: In Ref. 11 the discontinuous boundary condition was written incorrectly for the case $\tilde{\omega} > 0$.

Equations (4.2) and (4.3) are similar to the following equation

$$u_t = \frac{c_s}{(\gamma-1)\pi}\pi_t. \tag{5}$$

Equation (5) has been used in earlier work,[13,14] where the following physical interpretation was given:

At a boundary, Eq. (5) models a sound wave, moving into an infinite region of undisturbed flow. (6)

Specific boundary conditions at the four spatial boundaries will now be given.

(A) $\zeta = 0$ is assumed to be a solid boundary. An appropriate boundary condition is $\tilde{w} = 0$. One can then obtain θ and $\tilde{u}$ from Eqs. (3.1) and (3.2), while π can be calculated from the following equation:

$$\frac{c_s}{(\gamma-1)\pi}\pi_\tau - \tilde{w}_\tau = -\left(\frac{c_s}{(\gamma-1)\pi}G_2 - G_3\right). \tag{7.1}$$

Equation (7.1) represents the linearized characteristic variable which propagates information from $\zeta > 0$ to $\zeta = 0$.

(B) Because of Eq. (4.1), $\zeta = 1$ is a streamline and consequently one and only one boundary condition is required here. The three differential equations to be used are Eqs. (3.1) and (3.2), and the following characteristic equation:

$$\frac{c_s}{(\gamma-1)\pi}\pi_\tau + \tilde{w}_\tau = -\left(\frac{c_s}{(\gamma-1)\pi}G_2 + G_3\right). \tag{7.2}$$

Three upper boundary conditions will be considered.

(1) Equation (4.2): This equation was derived mathematically in Ref. 11 as the continuous boundary condition. The interpretation given by (6) is not entirely valid here because the derivative in Eq. (4.2) is with respect to τ and not to t. Thus, with this boundary condition, the floating top pushes a line of constant pressure (namely $\zeta = 1$) into the "undisturbed" region and then superimposes the change dictated by Eq. (4.2). In essence, the characteristic variable of

Eq. (7.1) remains constant as it propagates from $\zeta > 1$ to $\zeta = 1$; this, of course, ignores hydrostatic changes far above $\zeta = 1$.

(2) Equation (4.3): This equation was derived in Ref. 11 as the discontinuous boundary condition. The physical interpretation is that the flow at $\zeta = 1$ behaves as a weak compression wave moving into a region of relatively undisturbed flow. However, the assumption now is that the wave acts at the moving boundary with respect to the undisturbed hydrostatic pressure at that position. That is, the change dictated by Eq. (4.2) is imposed on the undisturbed region above $\zeta = 1$; the second term on the right in Eq. (4.3), for $\tilde{w} > 0$, accounts for the hydrostatic change in pressure. Interpretation (6) would seem, therefore, to be valid for this boundary condition.

(3) Both Eqs. (4.2) and (4.3) assume that the flow above $\zeta = 1$ is relatively undisturbed. There are situations where this physical assumption is clearly not justified. One such example would be that of an incoming lateral wave, with the assumption that the wave is also entering above the region of computation. A possible physical assumption for this flow would be as follows: The flow above $\zeta = 1$ propagates laterally in a one-dimensional fashion, without being significantly affected by the flow below $\zeta = 1$. This is modeled mathematically by Eq. (5) with interpretation (6). Transforming to τ, one obtains the following:

$$\pi_\tau = \frac{(\gamma - 1)\pi}{c_s}(\tilde{u}_\tau + \zeta_t \tilde{u}_\zeta) - \zeta_t \pi_\zeta. \tag{8}$$

(C) At the lateral boundaries, three boundary conditions are required for inflow and one otherwise (assuming subsonic flow). At a noninflow point Eq. (3.1) can be used along with the following linearized characteristic equations:

$$a\tilde{u}_\tau - \tilde{w}_\tau = -(aG_1 - G_3), \tag{9}$$

$$\tilde{u}_\tau \pm \frac{c_s(1 + a^2)^{1/2}}{(\gamma - 1)\pi}\pi_\tau + a\tilde{w}_\tau = -\left(G_1 \pm \frac{c_s(1 + a^2)^{1/2}}{(\gamma - 1)\pi}G_2 + aG_3\right). \tag{10}$$

In Eq. (10), the plus sign is used at $\eta = 1$ and the negative sign at $\eta = 0$. The additional boundary condition at the noninflow points will be either Eq. (8), with the same physical interpretation, or the condition $u = 0$.

At inflow points, Eq. (10)—with the appropriate sign—can be used, but three additional boundary conditions need to be specified. This is particularly troublesome for θ because of the fact that perturbations in θ propagate so slowly, namely at the flow velocity: the computational times to be considered in this paper are far less than the approximately 14 hours required to traverse 500 km at 10 m/sec. It was decided, therefore, to make the physical assumption that θ is not perturbed by the external flow. From Eq. (3.1) one sees that outside perturbations can enter the region only if $u\theta_\eta \neq 0$. Assuming that $\theta_\eta = 0$ at an inflow boundary point, the following equation is obtained:

$$\theta_\tau + r\theta_\zeta = 0. \tag{11}$$

In order to determine the remaining conditions, it is necessary to distinguish between "forced" inflow and "passive" inflow. Forced inflow, which represents physically an external flow being impressed on the region, can be modeled simply: Either velocity or pressure is specified. For purposes of the present paper, it was decided to specify velocity:

$$\tilde{u} = h_1(t,z), \tag{12.1}$$

$$\tilde{w} = h_2(t,z). \tag{12.2}$$

[Equations (10) and (11), then, essentially determine θ and π.] However, the second case, where flow is in effect pulled into the region because of internally produced gradients, is more complicated. One possible physical assumption would be that the wave enters as a sound wave normal to the surface. Mathematically, this translates to Eqs. (8) and $w = 0$.

Summarizing, Eq. (3) at interior points and the following equations at boundary points are assumed to define a well-posed mathematical formulation of a well-defined physical problem:

(i) $\zeta = 0$: $\tilde{w} = 0$, (3.1), (3.2), (7.1); (13.1)

(ii) $\zeta = 1$: (3.1), (3.2), (7.2), and one of [(4.2), (4.3), (8)]; (13.2)

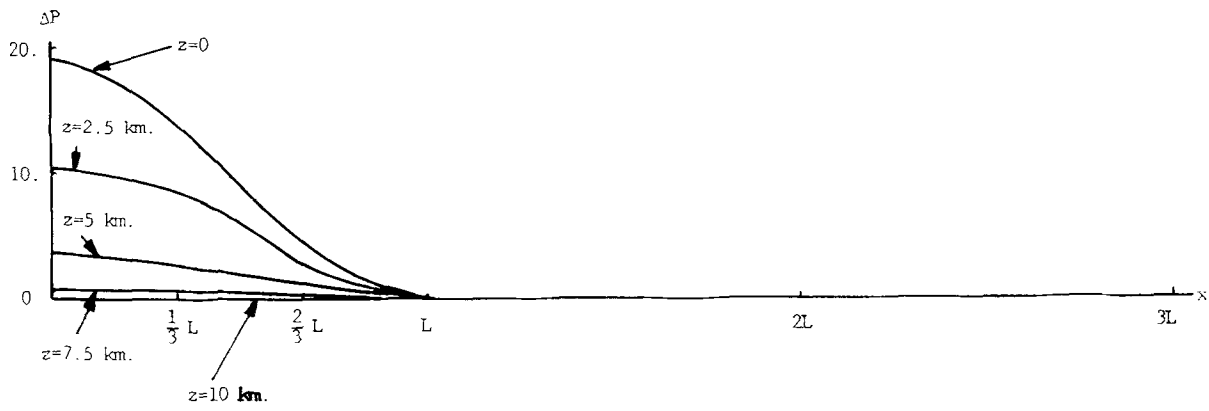

FIG. 2. Overpressure at initial time: $\Delta P = P(0,x,z) - P(0,L,z)$.

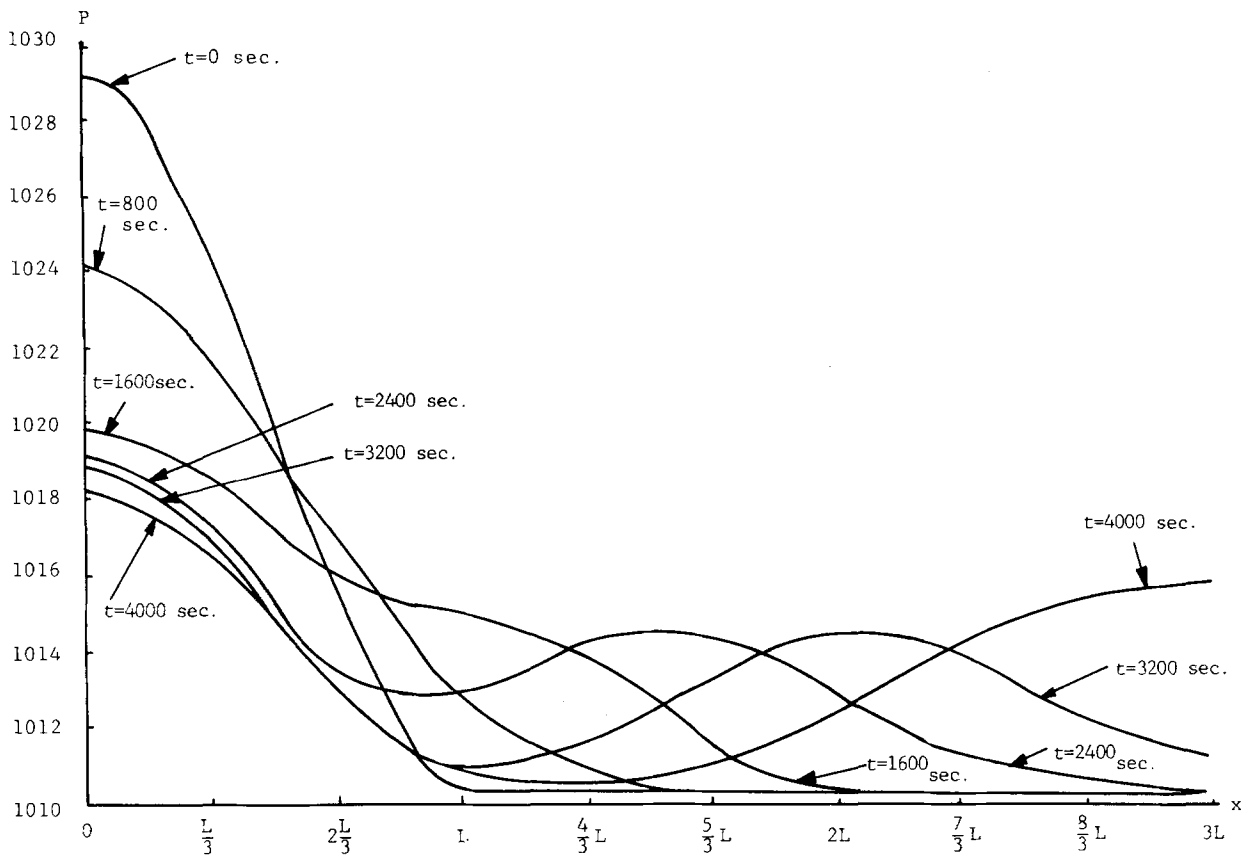

FIG. 3. $P(t,x,0)$.

(iii) $\eta = 0$ or 1:

(a) noninflow: (3.1), (9), (10), $u = 0$ (13.3)

or, (3.1), (9), (10), (8); (13.4)

(b) forced inflow: (10), (11), (12.1), (12.2); (13.5)

(c) passive inflow: (10), (11), (8), $w = 0$. (13.6)

The above formulation does not consider the corner points: $(\eta = 0,1; \zeta = 0,1)$. Several severe problems arise at these points:

(i) There are two sets of equations, corresponding to the two boundaries, that can be used. Generally, one attempts to use those relationships which are forcing the flow configuration. For example, an algebraic boundary condition, because of continuity requirements, is considered forcing.

(ii) Since the linearized characteristic equations are in general not valid, it may become necessary to use a partial differential equation directly. For example, if the flow is being forced at $\eta = 0$, $\zeta = 0$, then it is reasonable to impose Eqs. (12.1) and (12.2), with $h_2 = 0$, and to impose θ, say with Eq. (11), but one expects to calculate π from the internal flow. However, neither Eqs. (3.2) and (7.1), from the $\zeta = 0$ set, nor Eqs. (10) and (11) from the $\eta = 0$ set, can be applied. In this case one might be forced to use Eq. (3.3), $\pi_\tau = -G_2$, directly.

III. SPECIFICATION OF BOUNDARY CONDITIONS FOR THE QUASISTEADY MODEL

The quasisteady equations, obtained from Eq. (3) by assuming that π and $\tilde{w}$ are in quasisteady equilibrium with respect to θ and $\tilde{u}$, are as follows:

$$\theta_\tau = -r\theta_\zeta - (u/L)\theta_\eta, \quad \left.\begin{matrix}\\ \end{matrix}\right\} \text{unchanged} \tag{14.1}$$

$$\tilde{u}_\tau = -G_1, \tag{14.2}$$

$$G_2 = 0, \tag{14.3}$$

$$G_3 = 0. \tag{14.4}$$

It remains now to study the effect of the quasisteady assumption on the boundary conditions. The underlying principle is as follows:

If a boundary equation involves π_τ or $\tilde{w}_\tau$, and if the equation involves flow conditions internal to the region of computation, then the equation will be put in quasisteady equilibrium. (15)

At $\zeta = 0$ the situation is relatively simple. $\tilde{w} = 0$ and Eqs. (3.1) and (3.2) remain unaffected by the quasisteady assumption. According to (15), however, Eq. (7.1) becomes a quasisteady equation. This means that the right side of Eq. (7.1) is set to zero. Because of Eqs. (14.3) and (14.4), Eq. (7.1) is deleted from the system.

At $\zeta = 1$ a similar analysis holds: Equations (3.1) and (3.2) are still valid, while Eq. (7.2) is deleted. On the other hand, the upper boundary conditions are unaffected by the quasisteady assumption: Although involving quasisteady variables, these equations do not require internal conditions of the flow; in fact, the "derivation" of these equations was based on external flow conditions.

At the lateral boundaries a more complicated situation exists. First, note that Eqs. (14.3) and (14.4) were derived only at internal points of the flow and need not in principal be imposed at the boundaries. However, if these equations are not used at the lateral boundaries, the resulting solution may exhibit steep gradients. Such gradients will be inconsistent with the scale assumptions upon which the quasisteady equations are based. One concludes as follows:

The basic quasisteady assumption [Ref. 11, assumption 2] requires that Eqs. (14.3) and (14.4) be applied at all points of the lateral boundaries except possibly at the corner points. (16)

As noted in Ref. 11, the effect of the quasisteady equations, equations (14.3) and (14.4), is to remove internal time-dependence from the variables π and $\tilde{w}$. Boundary conditions must account for the time-dependence: $\tilde{w} = 0$ at $\zeta = 0$ accomplishes this for $\tilde{w}$ and the upper boundary condition provides the time-dependence for π. It is important to note that Eqs. (4.2) and (4.3) provide time-dependence relative to the upper flow, while Eq. (8) also relates to the external lateral flow; thereflow, if Eq. (8) is used at the top it is necessary to consider the possibility of incurring inconsistencies at the lateral boundaries.

Consider first noninflow points and assume the upper boundary condition is either Eq. (4.2) or (4.3). If the lateral equation set is given by (13.3), one would use Eqs. (3.1) and $u = 0$ for the quasisteady model, and if the lateral equation set is given by (13.4), one would use Eqs. (3.1) and (8). If the upper boundary condition is given by Eq. (8), the situation remains the same for equation set (13.3), but an inconsistency can arise with respect to equation set (13.4): Clearly, near $\zeta = 1$, Eq. (8) cannot be used to calculate $\tilde{u}$ "laterally" and π "vertically." In this case, since it seems reasonable to assume that $\tilde{u}$ can be obtained from the internal flow, Eq. (3.2) has been used directly (this assumes that the required time-dependence at the lateral boundary is provided by the upper boundary condition in conjunction with the quasisteady equations).

At forced inflow the situation is reasonably clear. Equation (10) is deleted from equation set (13.5) because it involves internal time derivatives of quasisteady variables, and the algebraic equation (12.2) is deleted because it is inconsistent with the quasisteady equation, Eq. (14.3). The remaining equations, Eq. (11) and (12.2), are used with the quasisteady model.

At passive inflow points Eq. (11) can still be applied in the quasisteady case. As above, Eqs. (10) and $w = 0$ are deleted. The remaining equation of equation set (13.6), namely Eq. (8), can be used if the upper boundary condition is given by Eq. (4.2) or (4.3). If the upper boundary condition is given by Eq. (8), then the same inconsistency, as discussed above, can arise if Eq. (8) is also used at the lateral boundary. This situation has not yet been resolved. One possible solution might be to again use Eq. (3.2) for $\tilde{u}$ [perhaps it is in some sense the "residue" of the quasisteady limit process relative to Eq. (10)]. Further study is required for this case.

TABLE I.

Top boundary Condition	non-inflow	forced inflow	passive inflow
(4.2) or (4.3)	(3.1), $u = 0$ or (3.1), (8)	(11), (12.1)	(11), (8)
(8)	(3.1), $u = 0$ or (3.1), (3.2)	(11), (12.1)	(11), ?

Summarizing, the quasisteady model consists of Eqs. (14.3) and (14.4) at all points and Eqs. (14.1) and (14.2) at all points except possibly $\eta = 0$ or 1. $\tilde{w} = 0$ is imposed at $\zeta = 0$. The additional feasible boundary conditions to be used in conjunction with these equations are summarized in Table I.

IV. INTERNALLY GENERATED OUTFLOW AND INFLOW

The numerical scheme is described in Ref. 11. All boundary conditions are solved implicitly (that is, at the forward time step). For example, at a lateral boundary Eq. (3.2) would be differenced as, $(1/\Delta t)(u_{i,j}^{n+1} - u_{i,j}^{n}) = -(G_1)_{i,j}^{n+1}$, where one-sided differences would be used as required. Since Eqs. (14.3) and (14.4) are also solved implicitly, the iteration problem becomes complicated.

The initial data used for the test problems in Ref. 11 consisted of a stationary flow with a lateral pressure gradient in a region of height h and length L. Because the lateral boundaries were assumed to be solid walls ($u = 0$ was the boundary condition), the flow, thereby generated, proceeded to reflect from the boundaries. In the present study, the right boundary will be a free boundary. The lateral boundary conditions must therefore allow the flow to move through and then, as it turns out, to move back into the region. These results will be compared with the following test case: The region is tripled to length $3L$, initial data in $0 \leqslant x \leqslant L$ is as above, data for the additional region is stationary flow with no pressure gradient. This latter problem is solved with the quasisteady model and $u = 0$ at the lateral boundaries. During a reasonably long time period, during which the results at $x = L$ are independent of the boundary conditions imposed at $x = 3L$, the results obtained with the large region can be compared with the free boundary case.

The initial flow field, for the region $0 \leqslant x \leqslant 480$ km $= L$, is as shown in Fig. 1 (this is reproduced from Ref. 11). $\tilde{w}$ and $\tilde{u}$ are zero throughout at time zero. Overpressure, with no pressure gradient in $L < x < 3L$, is shown in Fig. 2. For this test case, the continuous upper boundary condition, Eq. (4.2), was used at $\zeta = 1$, and $u = 0$ was imposed at $\eta = 0$ and 1. Figure 3 shows pressure at $z = 0$ for various times. Initially a "secondary" pressure front forms near $x = L$ (this can be seen at $t = 1600$), but by 2400 sec this front is moving toward the right boundary. This pressure distribution is accompa-

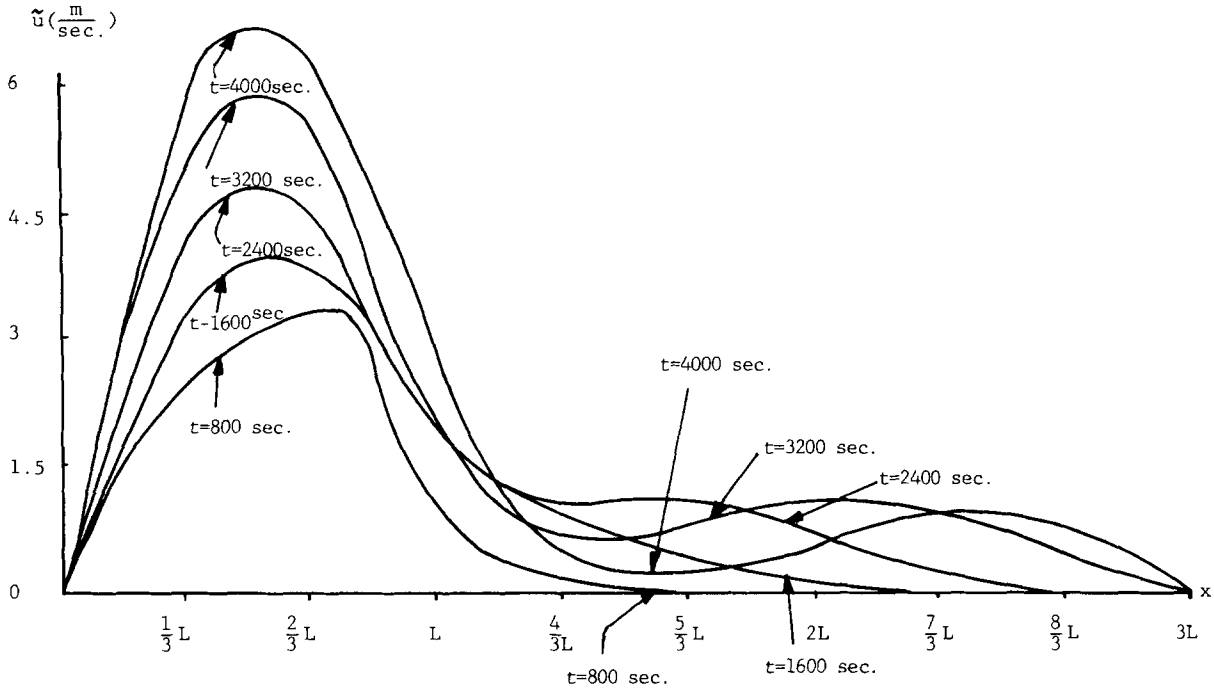

FIG. 4. $\tilde{u}$ AT $z = 0$; $\tilde{u}(t,0,x)$.

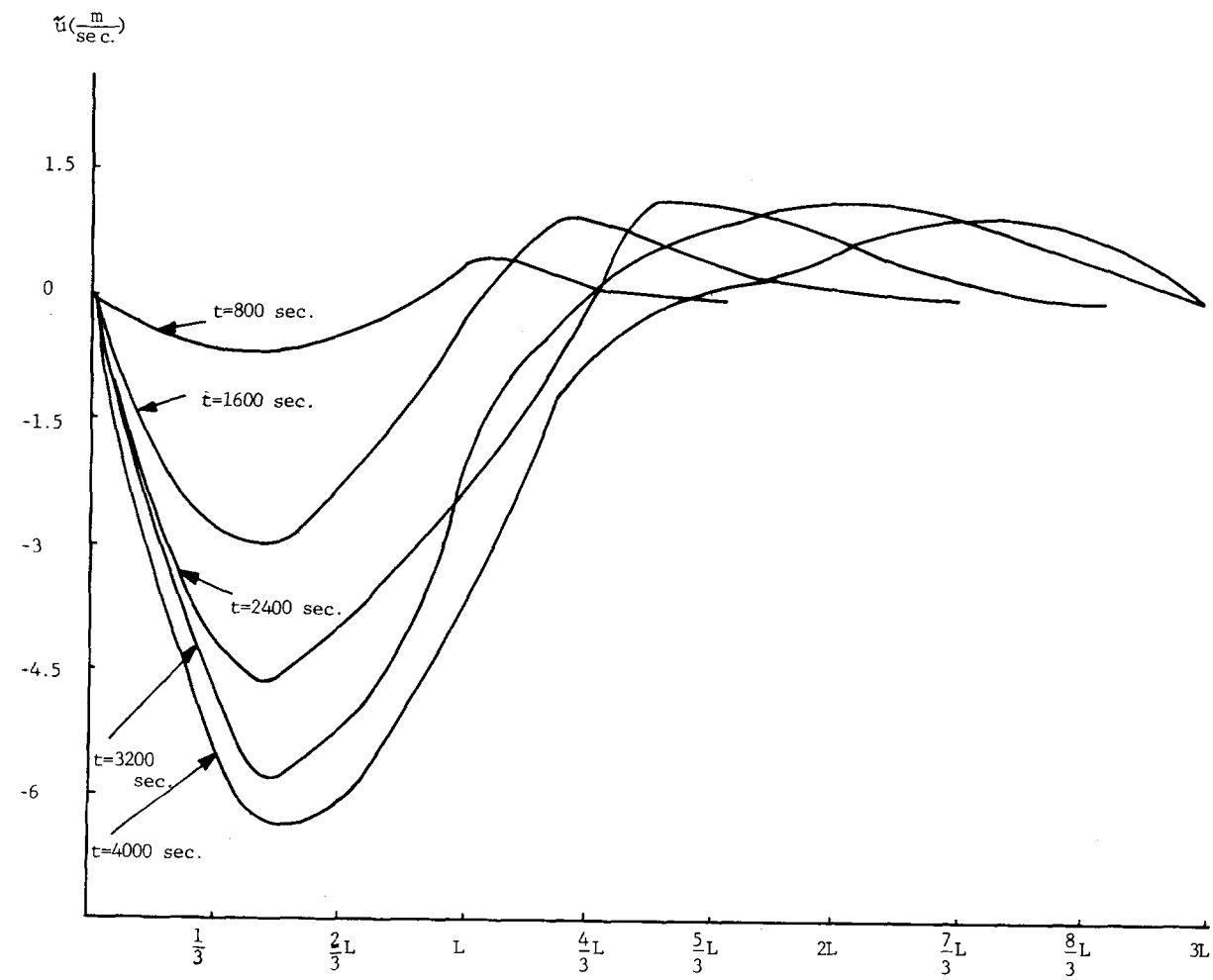

FIG. 5. $\tilde{u}$ at top surface.

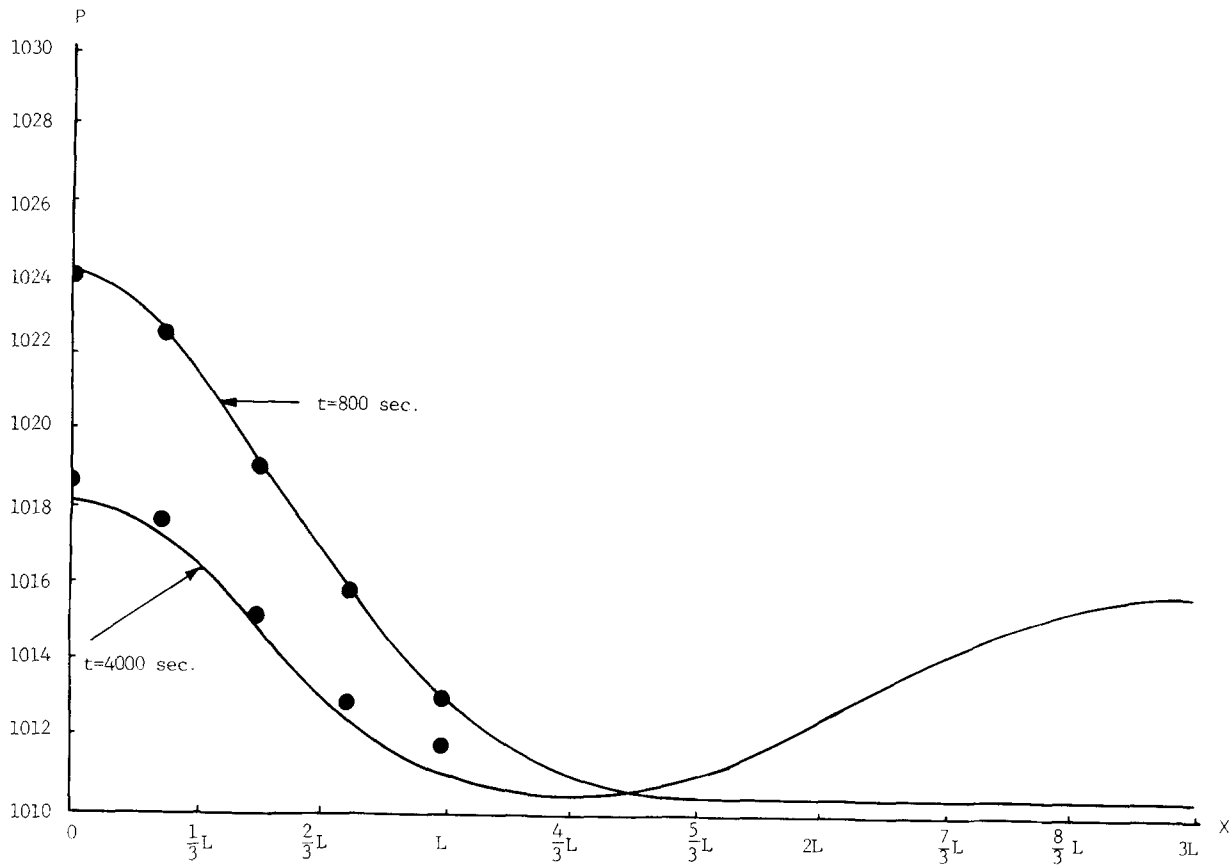

FIG. 6. Lateral boundary condition comparison for P.

nied by a reverse flow; this can be seen from Figs. 4 and 5, which display the $\tilde{u}$ distribution at $\zeta = 0$ and $\zeta = 1$.

Ideally, one would now like to specify boundary conditions at $x = L$ so that the solution thereby obtained would reproduce the above flow in $0 \leqslant x \leqslant L$. It seems fairly clear that for a problem of this complexity, such a goal cannot be attained. Nevertheless, because the flow is internally generated, one can expect to obtain the following with proper boundary conditions:

(a) The flow should be qualitatively correct (in this case outflow and reverse flow should occur in a generally appropriate time scale).

(b) Quantitatively, the results should be comparable.

If inflow occurs, it will be passive inflow. Thus, the following boundary conditions are used (see Table I): at $x = \eta = 0$, $u = 0$ and Eq. (3.1), and at $x/L = \eta = 1$, Eqs. (8) and (11).

This solution was run until time 4000 sec. In Ref. 11 it was shown that the oscillation time for this boundary condition was approximately 1600 sec. This implies a wave velocity of $L/1600 \approx 300$ m/sec, or about 6400 sec would be required for the wave to travel from L to $3L$ and back. It was felt, therefore, that for this time period the results should be independent of the boundary condition at $x = 3L$.

Boundary condition (8) is intended to represent a situation in which the external flow is undisturbed. Clearly, for this problem this assumption is not valid near $x = L$. However, it perhaps is satisfied for the flow sufficiently distant from $x = L$.

Figure 6 compares the pressure distribution at two times. The solid dots are the results using Eq. (8) at $x = L$. At time 800 sec the comparison is very good, while at time 4000 sec some discrepancy can be seen. Figure 7 shows the comparison in $\tilde{u}$ at the top surface. The effect of Eq. (8) seems to be to delay somewhat the development of reverse flow. The author judges this comparison to be good: In addition to maintaining the time scale of the problem, the results remain reasonable quantitatively also: It might perhaps also be noted that this is considered to be a difficult test case, particularly because of the combined inflow-outflow configuration at $x = L$.

This problem was also used to study the effect of underspecifying boundary conditions for the quasisteady equations, Eq. (14) This was accomplished by repeating the calculation (for the 480 km region) with the differential equation (14.2) replacing the boundary condition Eq. (8) at $\eta = 1$. The results, not shown, were sensible numerically, but agree very poorly with the results obtained with the large region. For example, at time 4000 sec, the pressure distribution has oscillated back essentially to the distribution existing at time 800 sec.

V. BELL-WAVE INPUT AT LEFT BOUNDARY

For this case the initial flow is stationary and hydrostatic: $\tilde{u} \equiv \tilde{w} \equiv 0$, $\partial\pi/\partial z = -(\gamma - 1)g/c_0^2\theta$, $\theta(0,x,z) = \theta(0,0,z)$ and $\theta(0,0,z)$ is as in the test case of Sec. IV [11, Eq. (22.8)]. At

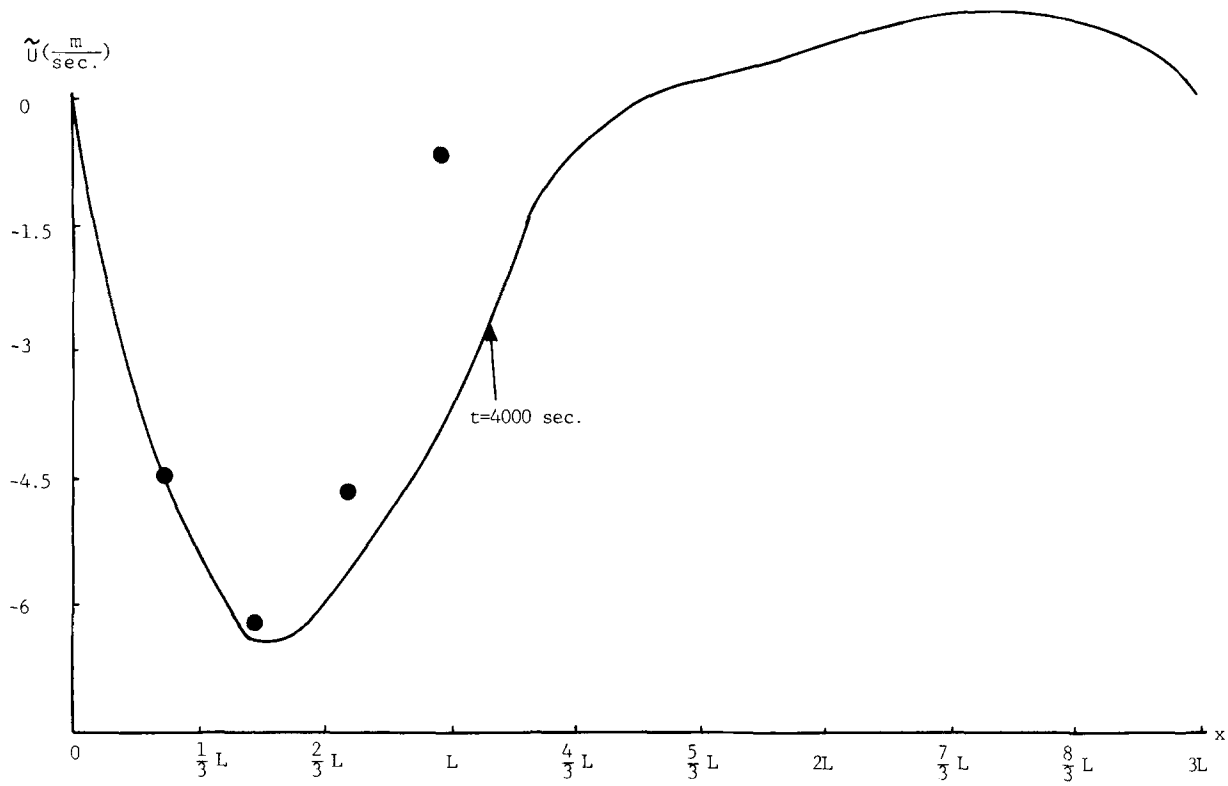

FIG. 7. Lateral boundary condition comparison for $\tilde{u}$ at top surfaces.

$x = 0$, $\tilde{u}$ is specified as a function of time:

$$\tilde{u}(\tau,0,\zeta) = \begin{cases} 16u_{\max}\left(\frac{\tau}{c_1}\right)^2\left(1-\frac{\tau}{c_1}\right)^2: & 0<\tau<c_1 \\ 0: & t>c_1. \end{cases} \tag{17}$$

$\tilde{u}$ thereby achieves a maximum of $u_{\max}$ at $\tau = c_1/2$.

The first calculation uses Eq. (8) at the upper boundary. Consequently, from Table I, Eq. (11) and (12.1) were imposed at $\eta = 0$ and Eqs. (3.1) and (3.2) at $\eta = 1$ (note that inflow at $\eta = 1$ does not occur for this case). The values of $u_{\max}$ and c_1 were taken respectively as 2.5 and 3200. Figure 8

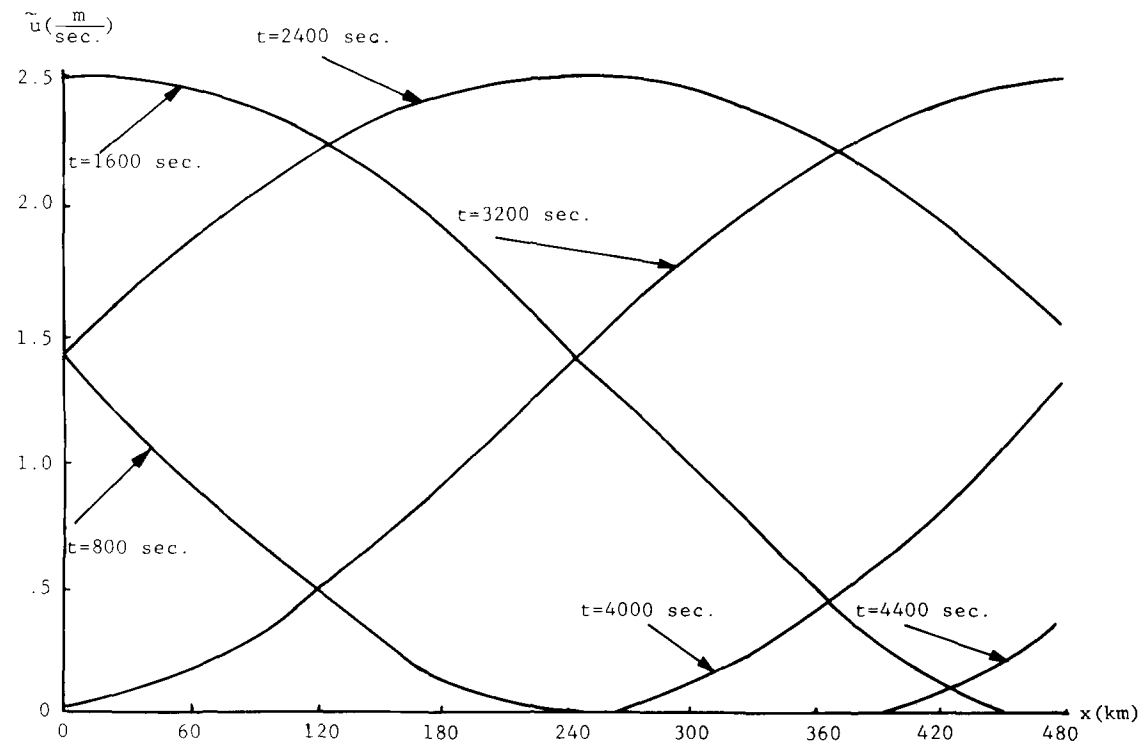

FIG. 8. Bell-wave input with upper boundary condition Eq. (8).

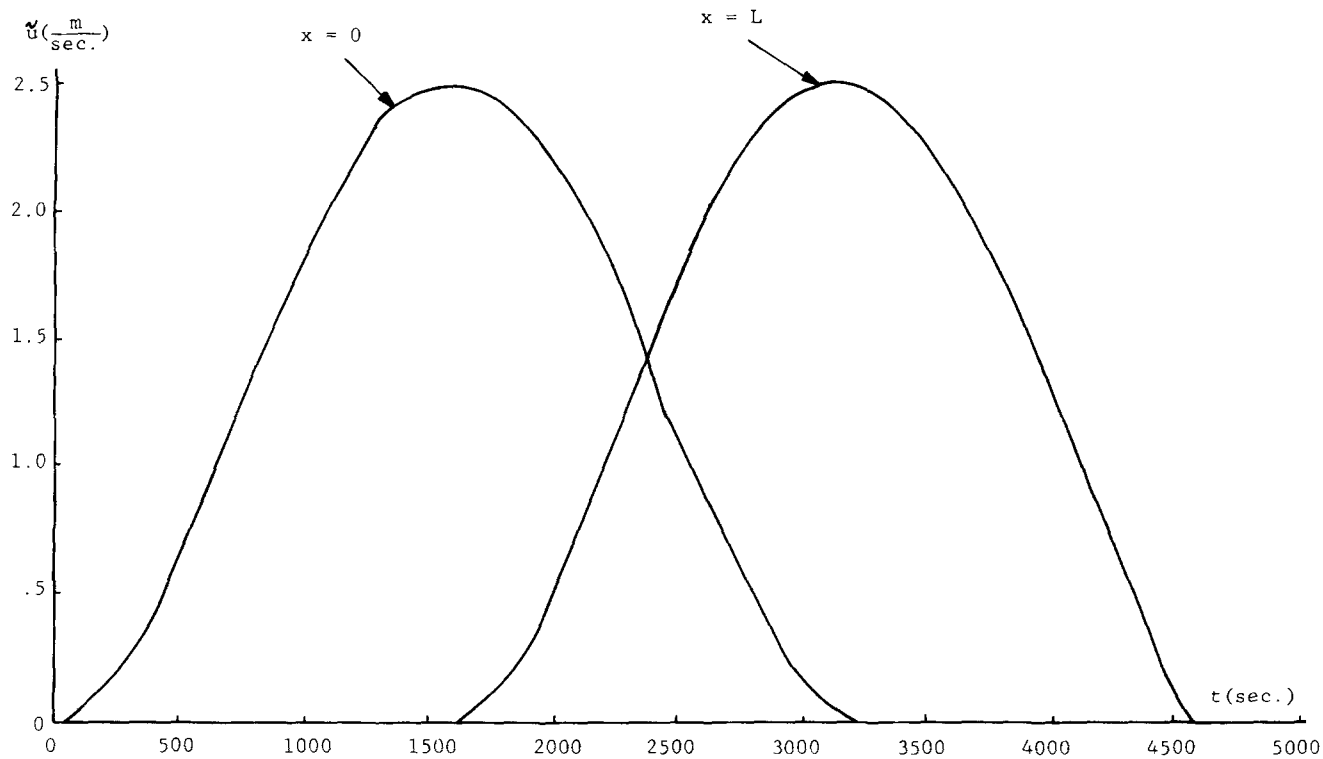

FIG. 9. $\tilde{u}$ at lateral boundaries for upper boundary condition Eq. (8).

shows the velocity distribution at the top surface for various times. At time 4800 sec this wave has left the region, and the flow, except for a small perturbation of approximately 4%, has returned to a stationary flow.

This residual flow, which apparently proceeds to oscillate back through the region with values $|\tilde{u}| < 0.1$ and $|\tilde{w}| < 0.005$, does not seem to be numerical error. Rather, it appears to be related to the difficulty noted in Sec. II of

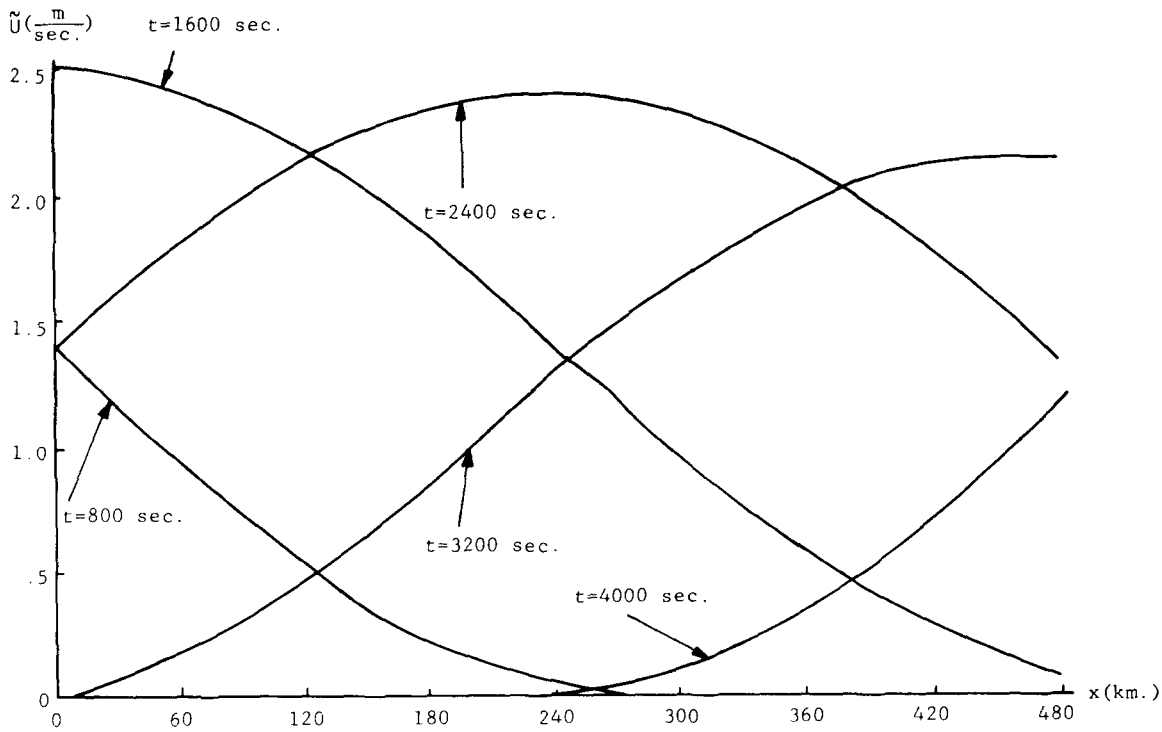

FIG. 10. Horizontal velocity at $\zeta = 0$ for upper boundary condition (4.2).

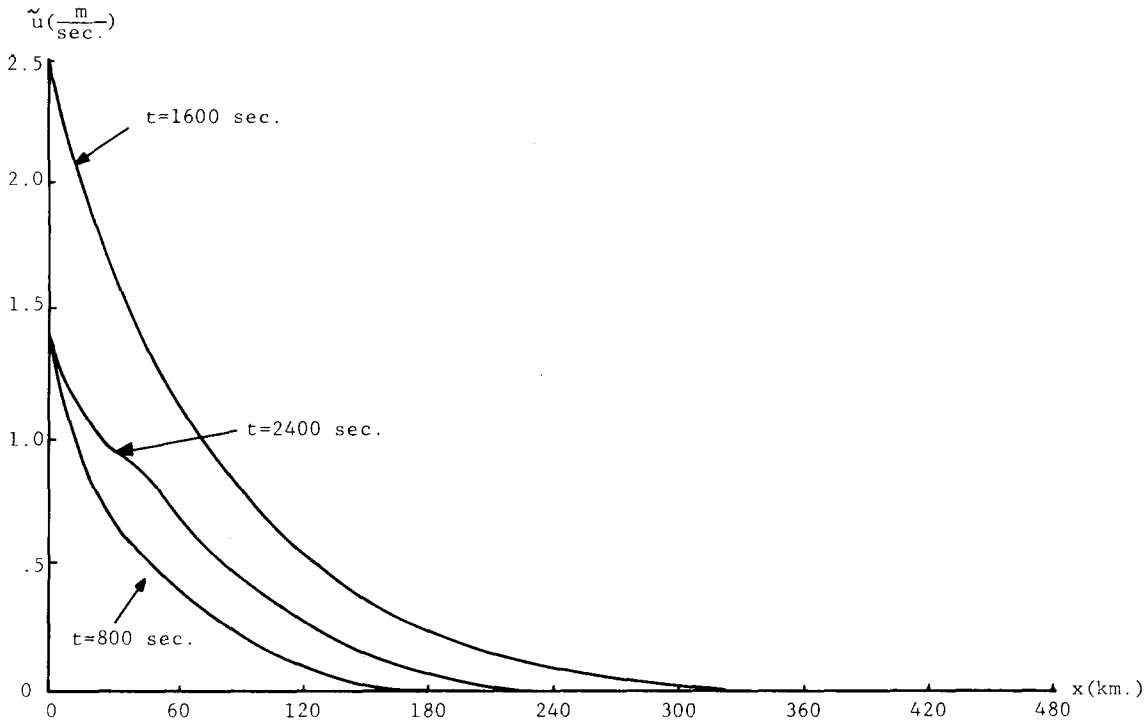

FIG. 11. Bell-wave input with upper boundary condition (4.3).

achieving a true steady-state solution. This difficulty is due to the slow time scale of θ. At time 6000 sec, the variation of θ from its values at time zero is still on the order of 10^{-4}; this is sufficient to maintain pressure gradients to account for the values noted above. To partially check this statement, the calculation was repeated with θ held constant throughout the region ($\theta \equiv \theta_0 = 1.05$). The "residual" values of velocity in this case were $|\tilde{u}| < 0.001$ and $|\tilde{w}| < 0.0001$.

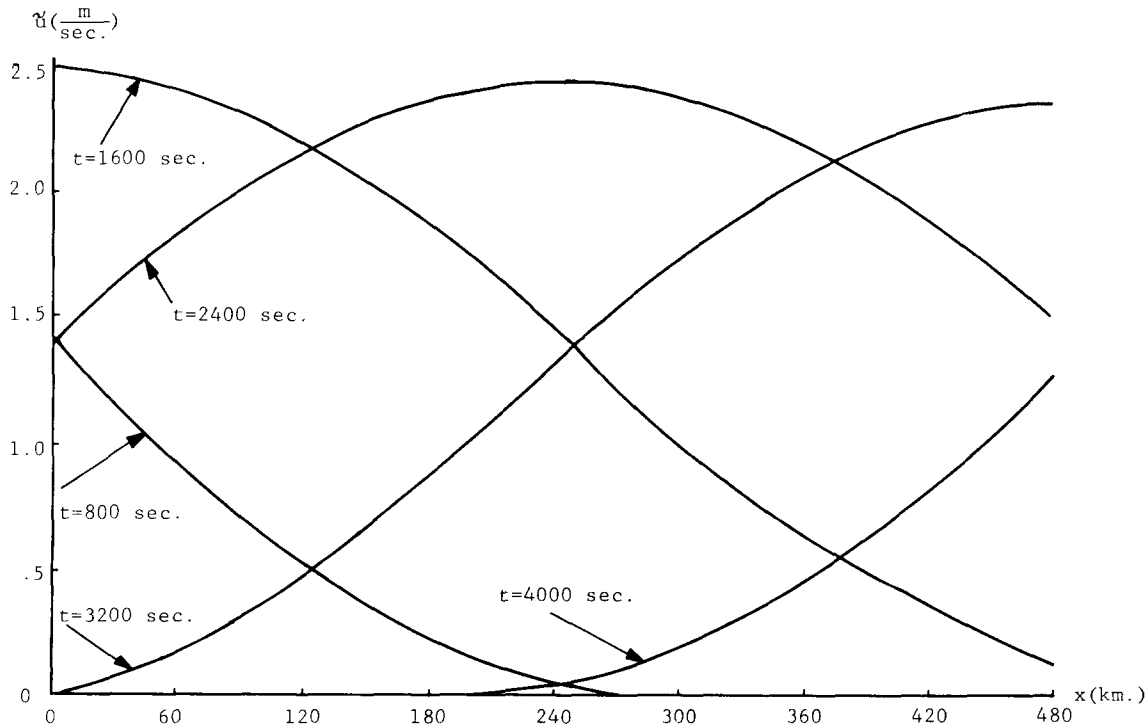

FIG. 12. Combined upper boundary condition.

The shape of the wave form, as a function of time, is shown in Fig. 9. The curve labeled $x = 0$ represents Eq. (17) for the conditions given above. The curve labeled $x = L$ represents the velocity curve as it exits the region at the upper boundary. Since the region was initially in equilibrium, one expects the wave to move through relatively unchanged. The curve shown in Fig. 9 indicates that this is the case. In addition, there is no damping of the wave. The exiting velocity curve at $z = 0$ is similar to that shown in Fig. 9, except that the maximum value is 2.288.

This problem was next solved with the other two upper boundary conditions. From Table I, Eqs. (11) and (12.1) are used at $\eta = 0$ and Eqs. (3.1) and (8) are used at $\eta = 1$. Again, the shape of the curve is maintained well. The vertical distribution is somewhat more pronounced for this case. For example, the maximum outflow velocity at $\zeta = 0$ is $\tilde{u} = 2.151$, while the maximum value of $\tilde{u}$ at $\zeta = 1$ is 2.505. Figure 10 shows the horizontal velocity distribution at $\zeta = 0$ for various times.

For the discontinuous boundary condition, Eq. (4.3), the results are markedly different. Since a small pressure gradient is maintained at the top surface, horizontal velocity falls off rapidly at the top. In fact, as noted in Fig. 11, the wave does not reach the far boundary, but instead decays rapidly. This would indicate that a large amount of energy is being dissipated to the outside upper region. Velocity at $\zeta = 0$ does build up more completely: The maximum value of $\tilde{u}$ at ($\zeta = 0$, $\eta = 1/2$) is 1.5 and occurs at time 2800 sec, while the maximum value at the right boundary ($\zeta = 0$, $\eta = 1$) is .1 and occurs at time 3800 sec. By time 4800 sec, a complete reverse flow exists.

It is also of interest to consider an upper boundary condition containing both a horizontal and vertical effect. One such equation, obtained by adding the right-hand sides of Eqs. (4.2) and (8), is the following:

$$\pi_\tau = \frac{(\gamma-1)\pi}{c_s}\tilde{w}_\tau + \frac{(\gamma-1)\pi}{c_s}(\tilde{u}_\tau + \zeta_\tau \tilde{u}_\zeta) - \zeta_\tau \pi_\zeta. \tag{18}$$

The physical interpretation of Eq. (18) is that the primarily one-dimensional flow propagating above $\zeta = 1$ [described by Eq. (8)] is perturbed by the vertically moving region [described by Eq. (4.2)].

Figure 12 shows results of the calculation using Eq. (18) at the top and Eqs. (3.1) and (3.2) at the right lateral boundary. It is seen that the wave form is much like that obtained with the individual equations (compare with Figs. 8 and 9). However, there is an important distinction in that Eq. (18) produces some damping of the wave form: The maximum value of $\tilde{u}$ at $\eta = 1$ is 2.36 and occurs at approximately $t = 3100$ sec. This damping appears to be totally an upper boundary effect, unrelated to the lateral boundaries: Note that the wave is already depressed by time 2400 sec. Also, comparison at an earlier time, before the wave has propagated into the region, shows no appreciable difference between the three cases Eq. (8), Eq. (4.2), and Eq. (18).

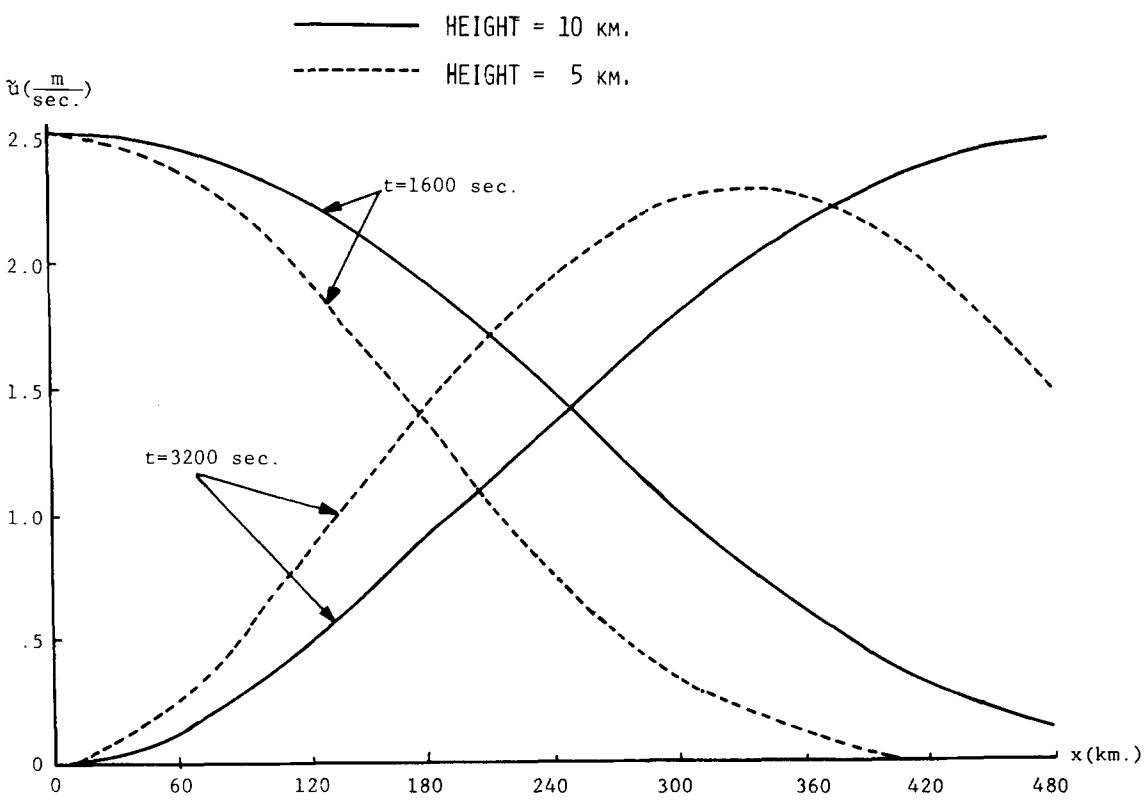

FIG. 13. Effect of height with upper boundary condition (4.2).

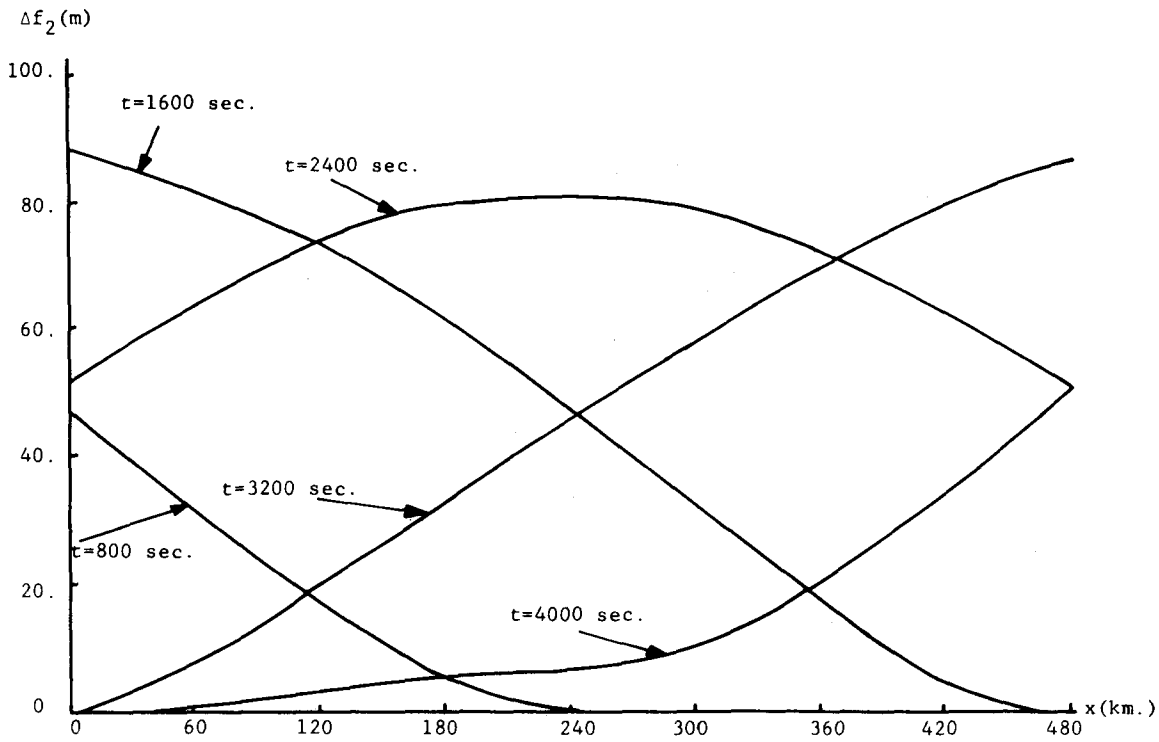

FIG. 14. Perturbation of the upper boundary for Eq. (8).

The three boundary conditions, Eqs. (4.2), (4.3), and (8), differ in another important characteristic, namely dependence on height. Equation (8) was "designed" to minimize this dependence: The physical assumption that the flow is also being imposed above $\zeta = 1$ indicates that the wave profile at $\zeta = 1$ should be relatively unaffected by the height of the lower region. This was verified by a calculation with a height of 5 km instead of 10 km. The other two boundary conditions, however, assume undisturbed flow above $\zeta = 1$ and consequently should be height dependent. This depen-

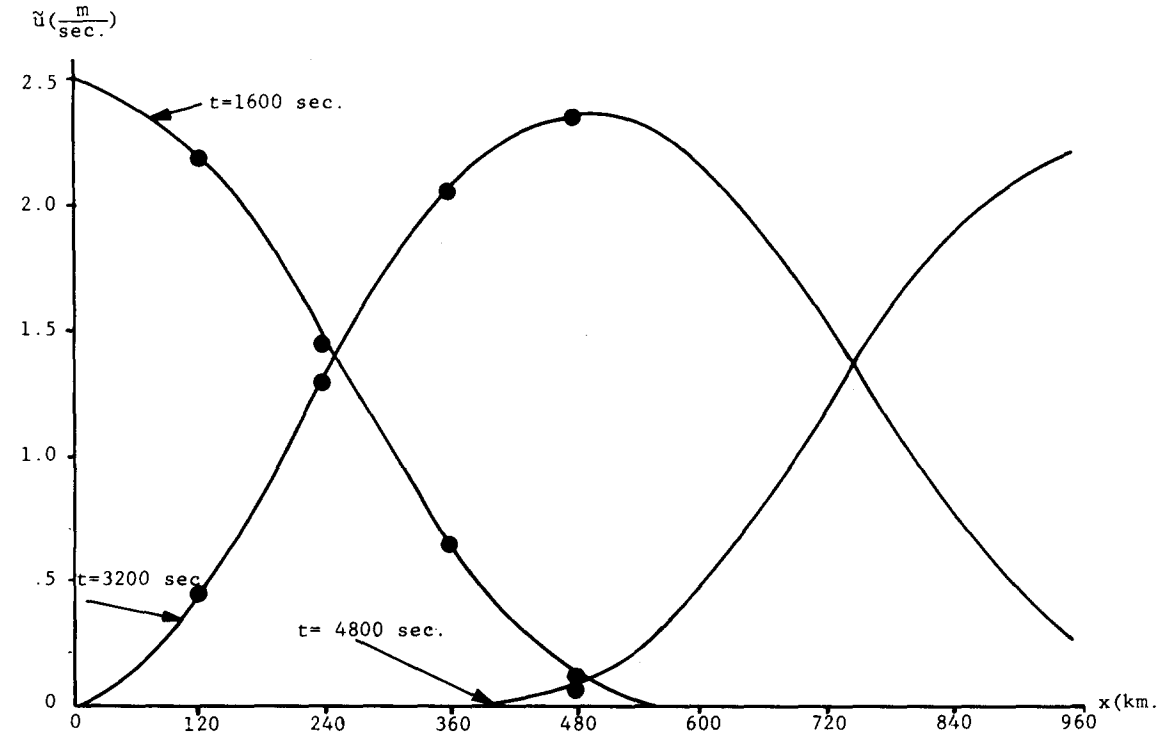

FIG. 15. Comparison with doubled length at $\zeta = 1$.

TABLE II.

	$\tilde{u}(\tau,\frac{1}{2},1)$	$\tilde{w}(\tau,\frac{1}{2},1)$	$\Delta f_2(\tau,0)$	$P(\tau,\frac{1}{2},0)$	$\theta(\tau,\frac{1}{2},\frac{1}{2})$
run 1	1.4634	0.0747	46.75	1034.448	0.0000064
run 2	1.4683	0.0739	46.42	1034.938	0.0000071
run 3	1.4694	0.0734	46.20	1035.078	0.0000075
Δ 1	− 0.0049	0.0008	0.33	− 0.490	− 0.0000007
Δ 2	− 0.0011	0.0005	0.22	− 0.140	− 0.0000004
Δ 2/Δ 1	− 0.224	0.625	0.667	0.286	− 0.57

dence is reflected in the form of the equations: Equations (4.2) and (4.3) involve vertical velocity, which is a quantity very sensitive to height.

Figure 13 compares two calculations, with the heights of 10 km and 5 km respectively, both using Eq. (4.2) at the top and the same lateral boundary conditions as discussed earlier. Two features of the flow are particularly interesting:

1) The smaller region propagates the wave more slowly. This is perhaps as expected, since vertical velocity is smaller and consequently pressure builds up more slowly.

2) There is a damping effect related to height. The 5 km case produced a maximum outlet velocity of 1.89 m/sec, while for the 10 km case the maximum outlet velocity was shown to be 2.505. Perhaps for this combination of wave input and boundary condition the height of 10 km is some kind of "magic number": At this height the wave propagates across the field in a relatively unpertubed manner. Clearly, there is a significant mathematical relationship between the wave input, the height of the region, and the upper boundary condition. At the present time, what one requires here is a physical explanation of this relationship.

As discussed in Ref. 11, the floating top is an important part of the model. Figure 14 displays the motion of the top for the case with Eq. (8) as the upper boundary condition. In general this motion parallels the velocity profile, as can be seen by comparing with Fig. 8. This was also true for the cases of boundary conditions (4.2) and (18). The maximum perturbation for each of the three cases [using Eq. (8), (4.2), and (18) respectively] was 87.6 m, 81.75 m, and 87.4 m. For the discontinuous boundary condition, Eq. (4.3), the top boundary rose 241.5 m.

As in the test case of Sec. IV, the lateral boundary conditions were tested by increasing the length of the region. The region was doubled in length, with the boundary conditions formerly imposed at $x = L$ now being imposed at $x = 2L$. Figures 15 and 16 show typical results of this investigation. This particular data is from the case with upper boundary condition (18) and right lateral conditions given by Eqs. (3.1) and (3.2). The solid lines are the results obtained with the doubled length, while the solid dots are the results with the original length of 480 km. The agreement at $\zeta = 1$ is very good, while some discrepancy builds up at $\zeta = 0$. The author concludes that these calculations give strong assurance that the lateral boundary conditions, in conjunction with the given upper boundary condition, are consistently modeling the hypothesized physical situation. In this case, the hypothesized physical situation is that of an external flow which is undisturbed "sufficiently far" from the region of interest.

Accuracy of the computations, relative to mesh size, is considered to be an important part of a numerical study. Of the three classes or problems discussed in this paper, the bell-wave problem of this section displayed the steepest gradients and consequently also displayed the greatest difficulty in establishing convergence.

As discussed in Ref. 11, one should at least be able to demonstrate that the solutions of a numerical algorithm behave as though they are part of a convergent sequence of calculations. For a first order method the following criterion was derived in Ref. 11:

$$\Delta 2/\Delta 1 \leqslant 0.5, \tag{19}$$

where $\Delta 1 = f^*(\tau,\eta,\zeta,h) - f^*(\tau,\eta,\zeta,h/2)$, $\Delta 2 = f^*(\tau,\eta,\zeta,h/2) - f^*(\tau,\eta,\zeta,h/4)$, and $f^*(\tau,\eta,\zeta,h)$ is the numerical approximation, obtained with step-size h, to the variable $f(\tau,\eta,\zeta)$.

For the problem using Eq. (8) at the upper boundary, the following sequence of calculations was made:

run 1: $\Delta x = 20$ km, $\Delta z \sim 1.25$ km, $\Delta t = 40$ sec,

run 2: $\Delta x = 10$ km, $\Delta z \sim 0.625$ km, $\Delta t = 20$ sec,

TABLE III.

	$\tilde{u}(\tau,1,0)$	$\tilde{u}(\tau,1,1)$	$P(\tau,0,0)$	$P(\tau,0,1)$	$\tilde{w}(\tau,0,1)$
run 1	0.0054	0.0041	1038.503	268.697	0.0049
run 2	− 0.0002	− 0.0007	1038.915	268.730	0.0013
run 3	− 0.0011	− 0.0012	1039.014	268.757	0.0001
Δ 1	0.0056	0.0048	− 0.412	− 0.043	0.0036
Δ 2	0.0009	0.0005	− 0.099	− 0.027	0.0012
Δ 2/Δ 1	0.161	0.104	− 0.240	0.63	0.333

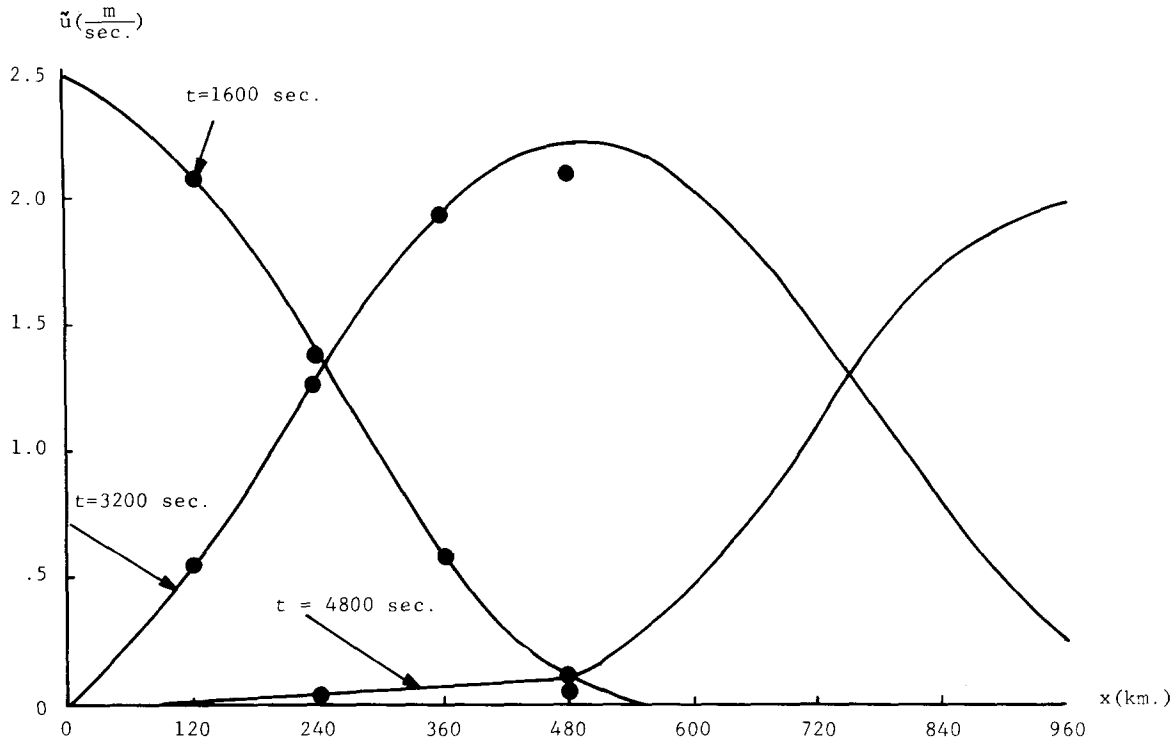

FIG. 16. Comparison with doubled length at $\zeta = 0$.

run 3: $\Delta x = 5$ km, $\Delta z \sim 0.3125$ km, $\Delta t = 10$ sec.

At time 1600 sec, Tables II and III display typical results for various quantities in the flow field.

In general, criterion (19) is satisfied very well. Δf_2 represents the actual motion of the top surface and θ represents the deviation of θ from its initial vlaue: In both these cases there is some question regarding the significance of the

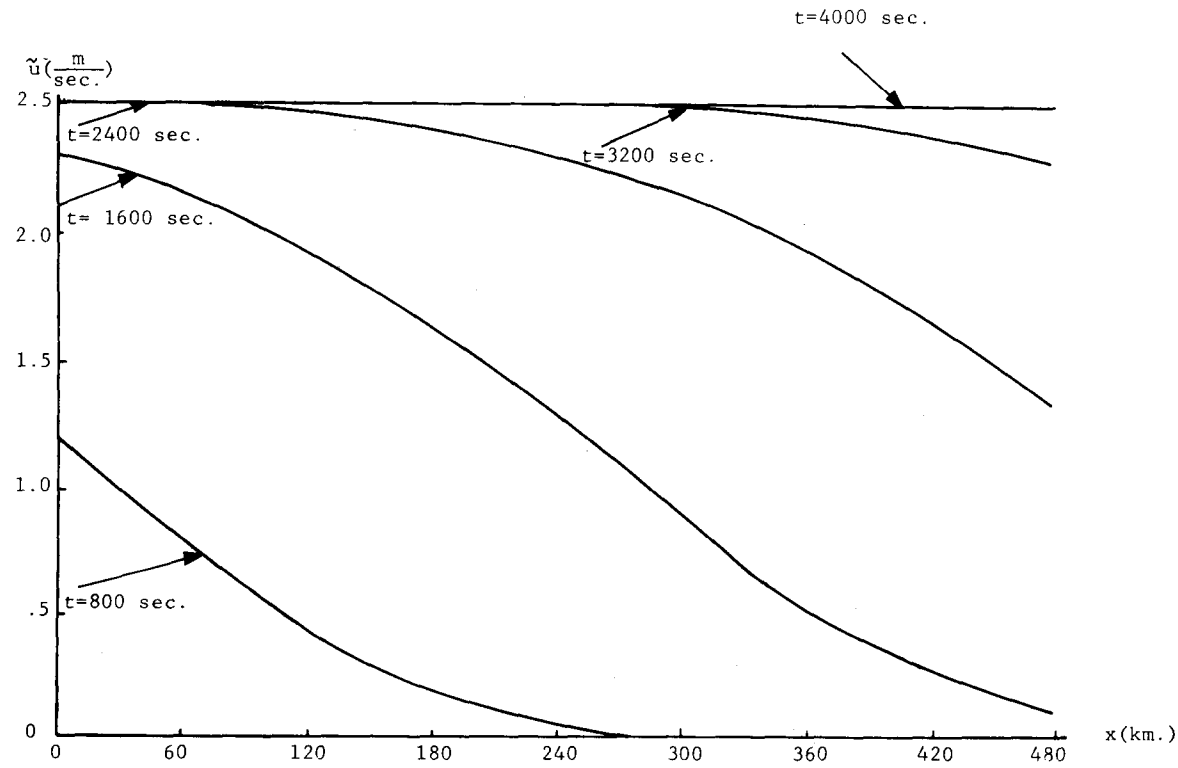

FIG. 17. Horizontal veloctiy at top surface.

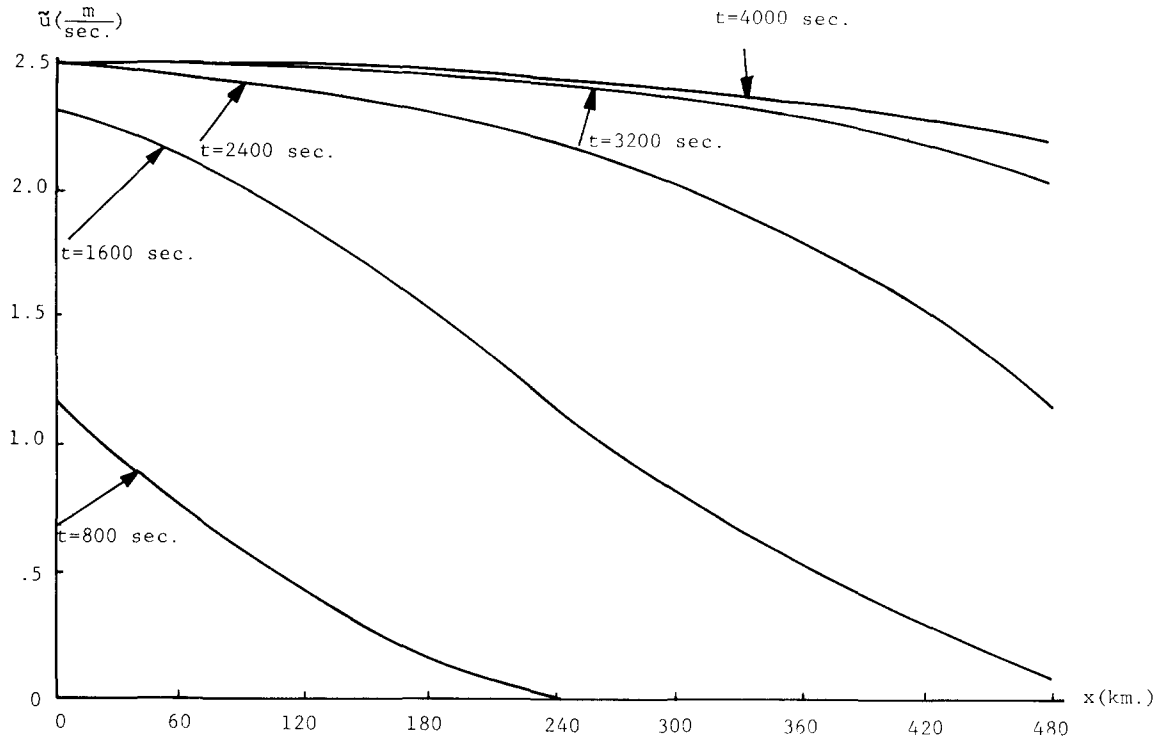

FIG. 18. Horizontal velocity at bottom surfaces.

digits shown in the table. Note also that $P(\tau,0,1)$ changes little from its initial value (namely 269.039), while $P(\tau,0,0)$ changes much more significantly (from its initial value of 1029.792).

VI. FLAT WAVE INPUT AT LEFT BOUNDARY

The problem is precisely as that discussed in Sec. V, except that Eq. (17), the input function for $\tilde{u}$, is replaced by the following:

$$\tilde{u}(\tau,0,\zeta) = u_{\max}[1 - \exp(-c_1 \tau^2)]. \tag{20}$$

For the sample calculation $u_{\max}$ was again 2.5 and $c_1 = 10^{-6}$. Using the upper boundary condition Eq. (8) and the lateral boundary conditions (at $\eta = 1$) Eqs. (3.1) and (3.2), one obtains the solution depicted in Figs. 17 and 18. The solution at the top surface is as expected: the velocity builds up, according to Eq. (20), and propagates across the field. However, the solution at $\zeta = 0$ was not expected, in that the maximum velocity at $\eta = 0$ did not propagate in the expected time scale. (By time 6000 sec, the profile changes little from that at time 4000 sec.) The "discrepancy" is approximately the same as that seen earlier in the bell-wave calculation.

It is clear, from simple conservation of mass considerations, that the solution as shown cannot be a steady-state solution. Calculations with reduced mesh size indicate that numerical error cannot account for the unexpected form of the solution. Also, one expects the error introduced by the quasisteady equations to be manifested, not in the final flow profiles, but in the short-term time scale. Relative to the time-scale of the problem, this error should be small.

Referring to Eq. (3.2), one sees that the π_η term is the most important factor in the propagation of $\tilde{u}$. The coefficient of this term involves only θ. A calculation with θ constant should, then, remove much of the vertical variation, but would not affect the quasisteady assumptions. Such a calculation was made, with $\theta = 1.05$. The velocity profiles are much like those of Fig. 17, except slightly retarded. However, there is no significant variation between the top and bottom horizontal velocity. Futhermore, this calculation achieves a steady-state: By time 4400 sec, the variation in the position of the top surface is 1.3 m (from $\eta = 0$ to $\eta = 1$), and the maximum value of $|\tilde{w}|$ is 0.0001.

A more careful analysis of the original calculation (with variable θ) shows that the solution, although not in steady-state, is very slowly varying. For example, at time 6000 sec the variation in the position of the top surface is 5.52 m, and the maximum value of $|\tilde{w}|$ is 0.0062. In light of the constant θ calculation, it would appear that the variables $\tilde{u}$, $\tilde{w}$, and π are in quasisteady equilibrium with respect to the θ field. (This problem of the slowly varying θ was discussed in Sec. II and Sec. V.)

VII. SUMMARY AND CONCLUSIONS

The primary goal of the paper was to develop a quasisteady model which 1) allowed inflow and outflow at lateral boundaries, and 2) was suitable for use in large-scale atmospheric flow.

The basic scale assumption, (Ref. 11, assumption 2) is the following:

Equation (3) is to be solved in a region of height h and length L, with $h \ll L$. It is assumed that boundary conditions

and initial conditions to be imposed on Eq. (3) are such that the flow variables will experience significant variations only over time scales which are large compared to h/c_s.

The analysis proceeded in two steps:

1) Boundary conditions were specified for the complete time-dependent equations, Eq. (3). In each case, an attempt was made to state the physical assumption being implied in regard to the external flow.

2) The above scale assumption was then applied consistently to both the partial differential equations and boundary conditions.

Several specific conclusions are as follows:

a) Because the numerical time step is not affected by vertical sound propagation, the quasisteady model operates on a time-scale suitable for large-scale atmospheric flow.

b) All solutions were shown to be stable and continuously dependent on the data. (In Ref. 11 it was indicated that convergence in terms of a decreasing mesh size is a test of stability.)

c) All solutions shown appear to have a sensible physical interpretation. However, in one problem (see Sec. VI) an overshoot occurred at a corner point; this might indicate that, for this choice of boundary conditions, the quasisteady limit was not taken correctly.

d) The proposed lateral boundary conditions behaved well and it was shown that they could be interpreted physically. In particular , the comparison with solutions for an extended region was very satisfactory.

e) In the problem of a wave entering at a lateral boundary, the profile of the propagating wave may be affected significantly, not only by the lateral boundary conditions, but also by the upper boundary condition and by the height of the region of entry.

f) Results with both the bell-wave input and flat-wave input indicate that, because of the slow reaction time for θ, in many cases steady-state solutions may not be achievable in physically realistic time scales. This behavior of θ needs to be factored into the physical interpretation of the problem.

ACKNOWLEDGMENTS

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Time evolution operator for N interacting quantum harmonic oscillators

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We discuss time evolution operator for N interacting quantum harmonic oscillators and determine certain conditions under which an explicit closed-form expression can be found for this time-ordered operator. The special case of $N = 2$ is discussed, as an example.

I. INTRODUCTION

In this paper, we discuss the time evolution of a system of N quantum harmonic oscillators interacting with each other. The Hamiltonian describing such a system, in the Schrödinger picture, is

$$\hat{H} = \sum_{\lambda,\mu=1}^{N} \omega_{\lambda\mu}(t)\hat{a}_\lambda^\dagger \hat{a}_\mu + \sum_{\lambda=1}^{N} [F_\lambda(t)\hat{a}_\lambda^\dagger + F_\lambda^*(t)\hat{a}_\lambda] + \beta(t) . \quad (1)$$

Here, as usual, the operators $\hat{a}_\lambda$, $\hat{a}_\lambda^\dagger$ are the annihilation and creation operators for the λ th oscillator and obey the commutation relations

$$[\hat{a}_\lambda, \hat{a}_\mu^\dagger] = \delta_{\lambda\mu} , \qquad [\hat{a}_\lambda, \hat{a}_\mu] = [\hat{a}_\lambda^\dagger, \hat{a}_\mu^\dagger] = 0 , \quad (2)$$

where $\lambda, \mu = 1, 2...N$. The time-dependent matrix $\omega_{\lambda\mu}(t)$ in (1) is Hermitian and $\beta(t)$ is real so that the Hamiltonian (1) is Hermitian. However, the coefficients $F_\lambda(t)$ are assumed to be arbitrary complex functions of time. Equation (1) gives the most general Hamiltonian for which a system, initially in a coherent state, will remain coherent for all times.[1]

In the Schrödinger picture, the state of the system at time t, $|\psi(t)\rangle$, is given by the relation

$$|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle , \quad (3)$$

where $|\psi(0)\rangle$ is the initial state of the system and the time evolution operator $\hat{U}(t)$ obeys the equation

$$i\hbar \frac{\partial \hat{U}}{\partial t} = \hat{H}\hat{U} . \quad (4)$$

The formal solution of Eq. (4) is

$$\hat{U}(t) = \left[\exp\left(-\frac{i}{\hbar}\int_0^t \hat{H}(t')\,dt'\right)\right]_+ , \quad (5)$$

where the subscript $+$ denotes the time-ordering operation defined by the relation[1,2]

$$\left[\exp\left(-\frac{i}{\hbar}\int_0^t \hat{H}(t')\,dt'\right)\right]_+ = 1 + \sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\right)^n\left[\int_0^t dt_1\cdots\int_0^t dt_n \hat{H}(t_1)\cdots\hat{H}(t_n)\right]_+ = 1 + \sum_{n=1}^{\infty}\left(-\frac{i}{\hbar}\right)^n \int_0^t dt_1\cdots\int_0^{t_{n-1}} dt_n \hat{H}(t_1)\cdots\hat{H}(t_n) . \quad (6)$$

An explicit expression can be found for the time-ordered operator $\hat{U}(t)$ if

$$[\hat{H}(t), \hat{H}(t')] = 0 , \quad (7)$$

i.e., if the Hamiltonian $\hat{H}(t)$ commutes with itself at another time t'. In such a case the expression (5) for $\hat{U}(t)$ simply reduces to

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\int_0^t \hat{H}(t')\,dt'\right) , \quad (8)$$

without the subscript $+$. However, in general, the commutation relation (7) may not hold. In such cases, it is difficult (and some times impossible) to obtain an explicit expression for $\hat{U}(t)$ without involving the time-ordering operation. In this paper, we give some conditions under which a closed-form explicit expression for the time-evolution operator $\hat{U}(t)$ for a system of N interacting quantum harmonic oscillators can be obtained.

The outline of the paper is as follows: In Sec. II, we eliminate the linear terms in the annihilation, creation operators $\hat{a}_\lambda$, $\hat{a}_\lambda^\dagger$ in the Hamiltonian (1) by translating the coordinate system. It is found that the time-dependent coefficients $c_\lambda(t)$ in the translation operator $T(t) = \exp[\Sigma_\lambda (c_\lambda(t)\hat{a}_\lambda^\dagger - c_\lambda^*(t)\hat{a}_\lambda)]$ obey first-order linear coupled differential equations. We determine conditions under which these equations can be solved. In Sec. III, we rotate the coordinate system and determine the conditions under which the new Hamiltonian (in the translated and rotated coordinate system) at time t commutes with itself at another time t'. One finds that these conditions are exactly the same as those required to determine the coefficients $c_\lambda(t)$ in the translation operator $\hat{T}(t)$ as treated in Sec. II. In Sec. IV, we discuss the case for $N = 2$, as an example, and also give some concluding remarks.

II. ELIMINATION OF LINEAR TERMS IN THE HAMILTONIAN (1)

In order to eliminate the linear terms in the annihilation and creation operators $\hat{a}_\lambda$, $\hat{a}_\lambda^\dagger$ respectively, we perform a transformation using the translation operator

$$\hat{T}(t) = \exp\left[\sum_{\lambda=1}^{N}(c_\lambda(t)\hat{a}_\lambda^\dagger - c_\lambda^*(t)\hat{a}_\lambda)\right], \quad (9)$$

where the time-dependent coefficients $c_\lambda(t)$'s are to be determined. In the new coordinate system, the equation of motion of the translated state vector

$$|\psi_T(t)\rangle = \hat{T}(t)|\psi(t)\rangle , \quad (10)$$

is given by

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$$i\hbar\frac{\partial}{\partial t}|\psi_T(t)\rangle = i\hbar\frac{\partial}{\partial t}[\hat{T}(t)|\psi(t)\rangle] = \hat{H}_T(t)|\psi_T(t)\rangle\,, \tag{11}$$

where the new Hamiltonian $\hat{H}_T(t)$ in the translated coordinate system is given by

$$\hat{H}_T(t) = i\hbar\frac{\partial\hat{T}}{\partial t}\hat{T}^{-1} + \hat{T}\hat{H}\hat{T}^{-1}\,. \tag{12}$$

The rhs of Eq. (12) can readily be calculated by using Eq. (9) and the relations

$$e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}} = e^{\alpha\hat{a}^\dagger}e^{-\alpha^*\hat{a}}e^{-(1/2)|\alpha|^2}\,,$$
$$\hat{T}\hat{a}_\lambda\hat{T}^{-1} = \hat{a}_\lambda - c_\lambda\,, \tag{13}$$

where α is an arbitrary c-number. We then obtain

$$\begin{aligned}\hat{H}_T(t) = {} & \sum_{\lambda\mu}\omega_{\lambda\mu}\hat{a}_\lambda^\dagger a_\mu \\ & + \sum_\lambda\Big[(i\hbar\dot{c}_\lambda - \sum_\mu\omega_{\lambda\mu}c_\mu + F_\lambda)\hat{a}_\lambda^\dagger + \text{c.c.}\Big] \\ & + \sum_{\lambda\mu}\omega_{\lambda\mu}c_\lambda^* c_\mu \\ & + \sum_\lambda[(\tfrac{1}{2}i\hbar\dot{c}_\lambda^* c_\lambda - F_\lambda^* c_\lambda) + \text{c.c.}] + \beta(t)\,.\end{aligned} \tag{14}$$

To eliminate the terms linear in $\hat{a}_\lambda$, $\hat{a}_\lambda^\dagger$, we choose the coefficients c_λ such that

$$i\hbar\dot{c}_\lambda(t) - \sum_\mu\omega_{\lambda\mu}(t)c_\mu(t) + F_\lambda(t) = 0\,. \tag{15}$$

Then, the Hamiltonian $\hat{H}_T(t)$ reduces to

$$\hat{H}_T(t) = \sum_{\lambda\mu}\omega_{\lambda\mu}(t)\hat{a}_\lambda^\dagger\hat{a}_\mu + \beta'(t)\,, \tag{16}$$

where

$$\beta'(t) = \beta(t) - \tfrac{1}{2}\sum_\lambda[F_\lambda^*(t)c_\lambda(t) + c.c.]\,. \tag{17}$$

The Hamiltonian (16) is free from the terms linear in the operators $\hat{a}_\lambda$, $\hat{a}_\lambda^\dagger$, but it contains $c_\lambda(t)$'s which are to be determined from N linear first-order, coupled differential equations (15) for which a closed-form solution may not always be possible. Therefore, before proceeding further, we first determine conditions under which the differential equations (15) can be solved.

We first observe that a formal solution of Eq. (15) is given by[3]

$$c_\lambda(t) = \sum_\mu P_{\lambda\mu}(t)c_\mu(0) + \frac{i}{\hbar}\sum_{\mu\sigma}P_{\lambda\mu}(t) \times\int_0^t P_{\sigma\mu}^*(t')F_\sigma(t')\,dt'\,, \tag{18}$$

where $P(t)$ satisfies

$$i\hbar\,\dot{P}_{\lambda\mu}(t) = \sum_\sigma\omega_{\lambda\sigma}(t)P_{\sigma\mu}(t)\,. \tag{19}$$

Hence if we can obtain an explicit expression for the time-ordered matrix

$$P(t) = \exp\Big[-\frac{i}{\hbar}\int_0^t\omega(t')\,dt'\Big]_+\,, \tag{20}$$

we can find $c_\lambda(t)$ using Eq. (18).

Next let us consider the equation

$$i\hbar\,\dot{G}_\lambda(t) = \sum_\mu\omega_{\lambda\mu}(t)G_\mu(t)\,, \tag{21}$$

and write

$$\omega_{\lambda\mu}(t) = |\omega_{\lambda\mu}(t)|e^{-i\theta_{\lambda\mu}(t)}\,. \tag{22}$$

Since $\omega_{\lambda\mu}$ is Hermitian, $|\omega_{\lambda\mu}|$ is symmetric and $\theta_{\lambda\mu}$ is antisymmetric in λ and μ. Let us assume that $\theta_{\lambda\mu}$ can be expressed as

$$\theta_{\lambda\mu}(t) = \theta_\lambda(t) - \theta_\mu(t)\,. \tag{23}$$

It may be observed that θ_λ's are arbitrary up to an additional scalar function of time. For definitiveness, we may write

$$\theta_1(t) = \tfrac{1}{2}\theta_{12}(t) + \theta(t), \tag{24}$$

where $\theta(t)$ is to be suitably chosen. The remaining θ_λ's can be determined from Eq. (23). Next, we set

$$B_\lambda(t) = \exp(i\theta_\lambda(t))G_\lambda(t)\,. \tag{25}$$

We then find from Eqs. (21)–(25) that

$$i\hbar\,\dot{B}_\lambda(t) = |\omega_{\lambda\mu}(t)|B_\mu(t) - \hbar\dot{\theta}_\lambda(t)B_\lambda(t)\,. \tag{26}$$

In matrix notation, Eq. (26) can be rewritten as

$$i\hbar\,\dot{B}(t) = W(t)B(t)\,, \tag{27}$$

where $B(t)$ is a column vector $\{B_\mu(t)\}$ and the matrix $W(t)$ is given by

$$W_{\lambda\mu}(t) = |\omega_{\lambda\mu}(t)| - \hbar\dot{\theta}_\lambda(t)\delta_{\lambda\mu}\,. \tag{28}$$

We may therefore obtain an explicit expression for $B(t)$ in case when $W(t)$ and $W(t')$ commute with each other, i.e., if

$$[W(t), W(t')] = 0\,. \tag{29}$$

It is often possible that the original matrix $\omega(t)$ does not commute with $\omega(t')$ and yet $W(t)$ has this property. It is readily seen that the condition (29) is identically satisfied if it is possible to diagonalize $W(t)$ by a time-independent orthogonal matrix M:

$$MW(t)M^{-1} = W_d(t)\,. \tag{30}$$

Hence we conclude that when the conditions (23) and (29) are satisfied, we may express Eq. (20) in the form

$$P_{\lambda\sigma}(t) = e^{-i[\theta_\lambda(t) - \theta_\lambda(0)]}(e^{-(i/\hbar)\int_0^t W(t')\,dt'})_{\lambda\sigma}\,, \tag{31}$$

and therefore obtain an explicit solution for $c_\lambda(t)$ as given by Eq. (18).

III. CLOSED-FORM EXPLICIT EXPRESSION FOR $\hat{U}(t)$

We have seen that the linear terms in the Hamiltonian (1) can be eliminated by translating the coordinate system using the operator $\hat{T}(t)$. The new Hamiltonian $\hat{H}_T(t)$ in the translated coordinate system is given by Eq. (16). In this section, we determine the general conditions under which an explicit expression for the time-ordered time-evolution operator $\hat{U}_T(t)$ for the Hamiltonian $\hat{H}_T(t)$ can be obtained.

We rotate our translated coordinate system using the rotation operator

$$\hat{R}(t) = \exp\Big(i\sum_\lambda\theta_\lambda\hat{a}_\lambda^\dagger\hat{a}_\lambda\Big)\,. \tag{32}$$

Then the equation of motion of the rotated state vector

$$|\psi_{RT}(t)\rangle = \hat{R}(t)|\psi_T(t)\rangle , \tag{33}$$

is given by

$$i\hbar\frac{\partial}{\partial t}|\psi_{RT}(t)\rangle = i\hbar\frac{\partial}{\partial t}[\hat{R}(t)|\psi_T(t)\rangle] = \hat{H}_{RT}(t)|\psi_{RT}(t)\rangle , \tag{34}$$

where

$$\hat{H}_{RT}(t) = i\hbar\frac{\partial\hat{R}}{\partial t}\hat{R}^{-1} + \hat{R}\hat{H}_T\hat{R}^{-1} . \tag{35}$$

The rhs of Eq. (35) is readily evaluated by using the relation

$$e^{-\alpha\hat{a}^\dagger\hat{a}}\hat{a}e^{-\alpha\hat{a}^\dagger\hat{a}} = \hat{a}e^{-\alpha} , \tag{36}$$

α being arbitrary c-number. We then obtain

$$\hat{H}_{RT}(t) = \sum_{\lambda\mu}\hat{a}_\lambda^\dagger W_{\lambda\mu}(t)\hat{a}_\mu + \beta'(t) , \tag{37}$$

where the matrix $W_{\lambda\mu}(t)$ is given by Eq. (28). It is readily verified that

$$[\hat{H}_{RT}(t), \hat{H}_{RT}(t')] = 0 , \tag{38}$$

under conditions (23) and (29). Therefore, the time-evolution operator $\hat{U}_{RT}(t)$ for the Hamiltonian can be put in an explicit closed form as follows:

$$\hat{U}_{RT}(t) = \exp\left[-\frac{i}{\hbar}\int_0^t \hat{H}_{RT}(t')\,dt'\right] . \tag{39}$$

The solution of Eq. (34) is then given by

$$|\psi_{RT}(t)\rangle = \hat{U}_{RT}(t)|\psi_{RT}(0)\rangle . \tag{40}$$

Using Eqs. (33) and (10) we may rewrite Eq. (40) in the form

$$|\psi(t)\rangle = \hat{T}^{-1}(t)\hat{R}^{-1}(t)\hat{U}_{RT}(t)\hat{R}(0)\hat{T}(0)|\psi(0)\rangle . \tag{41}$$

Thus, we find that an explicit expression for the time-evolution operator $\hat{U}(t)$ for the Hamiltonian (1) can be found under the conditions (23) and (29). The final expression for $\hat{U}(t)$ satisfying the relation (3) is then given by

$$\hat{U}(t) = \hat{T}^{-1}(t)\hat{R}^{-1}(t)\hat{U}_{RT}(t)\hat{R}(0)\hat{T}(0) , \tag{42}$$

where the operators $\hat{T}(t)$, $\hat{R}(t)$, and $\hat{U}_{RT}(t)$ are given by Eqs. (9), (32), and (39) respectively. Here it is to be noted that conditions (23) and (29) are independent of $F_\lambda(t)$'s and $\beta(t)$. It is also worth pointing out that the conditions under which we can obtain an explicit expression for $\hat{T}(t)$ which eliminates the linear terms in $\hat{H}$ are identical to those needed for obtaining an explicit expression of the time-evolution operator $\hat{U}_{RT}(t)$. In the next section, we consider the special case $N = 2$, and also give some general remarks.

IV. THE CASE $N = 2$ AND CONCLUDING REMARKS

The Hamiltonian we consider for a system of two quantum harmonic oscillators interacting with each other is given by

$$\hat{H}(t) = \sum_{\lambda,\mu=1}^{2}\omega_{\lambda\mu}(t)\hat{a}_\lambda^\dagger\hat{a}_\mu + \sum_{\lambda=1}^{2}[F_\lambda(t)\hat{a}_\lambda^\dagger + F_\lambda^*(t)\hat{a}_\lambda] + \beta(t) . \tag{43}$$

Here, as before, the matrix $\omega_{\lambda\mu}(t)$ is Hermitian, $\beta(t)$ is real and $F_\lambda(t)$'s are arbitrary complex functions of time.

We first observe that for the case $N = 2$, $\omega_{\lambda\mu}(t)$'s is a 2×2 matrix and $\theta_{11} = \theta_{22} = 0$, $\theta_{12} = -\theta_{21}$. Eq. (23) is then automatically satisfied and is not an extra requirement. For definitiveness, we write

$$\theta_1(t) = \tfrac{1}{2}\theta_{12}(t) + \theta(t) , \quad \text{[cf. Eq. (24)]}. \tag{44}$$

Next we consider the requirement (29). In this case

$$W(t) = \begin{pmatrix} \omega_{11}(t) - (\hbar/2)\dot{\theta}_{12}(t) - \dot{\theta}(t) & |\omega_{12}(t)| \\ |\omega_{12}(t)| & \omega_{22}(t) + (\hbar/2)\dot{\theta}_{12}(t) + \dot{\theta}(t) \end{pmatrix} . \tag{45}$$

As mentioned before, the condition (29) is identically satisfied if $W(t)$ can be diagonalized by a time-independent matrix. A less general condition is that $W(t)$ is a scalar function of time multiplied by a constant matrix

$$W(t) = f(t)W(0), \tag{46}$$

where $f(t)$ is a scalar function of time [with $f(0) = 1$]. It may be noted that $\theta(t)$ is still left for further manipulations. In particular if one of the eigenvectors of the matrix

$$W_0 = \begin{pmatrix} \omega_{11}(t) - (\hbar/2)\dot{\theta}_{12}(t) & |\omega_{12}(t)| \\ |\omega_{12}(t)| & \omega_{22}(t) + (\hbar/2)\dot{\theta}_{12}(t) \end{pmatrix} , \tag{47}$$

is constant, we may express $W(t)$ in the form (46) by setting $\dot{\theta}(t)$ to be equal to the eigenvalue of W_0 corresponding to the other eigenvector. This is readily seen by making use of the spectral representation[4] of W_0,

$$W_0 = \lambda_1 x_1 x_1^\dagger + \lambda_2 x_2 x_2^\dagger , \tag{48}$$

and the completeness relation

$$x_1 x_1^\dagger + x_2 x_2^\dagger = 1 , \tag{49}$$

where x_1 and x_2 are the eigenvectors of W_0 with the eigenvalues λ_1 and λ_2 respectively.

Hence we conclude that, for $N = 2$, if any one of the eigenvectors of the matrix W_0 given by Eq. (47), is constant, we can obtain an explicit expression for the time-evolution operator $\hat{U}(t)$.

A special case of the Hamiltonian (43), namely when $F_\lambda(t) = \beta(t) = 0$ and ω_{11}, ω_{22} time-independent, has been considered by Lu.[5]

Finally, it is worth mentioning again that there may be cases (for arbitrary values of N) in which the initial Hamiltonian $\hat{H}(t)$ does not commute with $\hat{H}(t')$ but the transformed Hamiltonian $\hat{H}_{RT}(t)$ exhibits this property. Consider, for example, the case when

$$\omega_{\lambda\mu}(t) = A_{\lambda\mu}\exp[\theta_\lambda(t) - \theta_\mu(t)] , \tag{50}$$

where

$$\theta_\lambda(t) = \nu_\lambda t + \phi_\lambda , \tag{51}$$

and $A_{\lambda\mu}$, ν_λ, and ϕ_λ are time-independent. In this case, it is readily verified that

$$[\hat{H}(t), \hat{H}(t')] \neq 0 ,$$

but the conditions (23) and (29) are satisfied so that the

transformed Hamiltonian $\hat{H}_{RT}(t)$ commutes with $\hat{H}_{RT}(t')$. Hence an explicit expression of the time-ordered unitary operator $\hat{U}(t)$ can be obtained in this case.

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Shift operator techniques for the classification of multipole-phonon states. VI. Properties of nonscalar R(3) product operators in the R($2\lambda+1$) groups

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Expressions connecting nonscalar R(3) products of operators which shift the eigenvalues of the R(3) Casimir operator L^2 are constructed within the R($2\lambda+1$) groups ($\lambda = 2$ or 3).

1. INTRODUCTION

In previous papers shift operators were constructed out of the enveloping algebra of the generators l_i ($i = 0, \pm$) of R(3) and the components of either a seven-dimensional tensor representation q_μ [1,2] or an eleven-dimensional tensor representation p_μ [3] of R(3). Those based upon q_μ are denoted as O_l^k, while the p_μ dependent ones are represented by P_l^k. Along the lines of the papers previously published by Hughes[4,5] on shift operator properties R(3) scalar product operators of the forms $O_{l+k}^{\ k}O_l^{+k}$ and $P_{l+k}^{-k}P_l^{+k}$ have been considered.[1-3] We could show further that a number of relations exist between these scalar quadratic operators and the other scalar operators available in the R($2\lambda+1$) groups ($\lambda = 2$ and 3) under consideration. We have established that in the four existing independent relations based upon $O_{l+k}^{-k}O_l^{+k}$ product operators four of the seven available quadratic forms are always present. For the P-type operator products six independent relations could be constructed, each composed of six of the eleven product operators.

By using the relations between the R(3) scalar products $O_{l+k}^{\ k}O_l^{+k}$, as derived for the R(5) group,[1] we were able to deduce the eigenvalues and corresponding eigenvectors of the R(3) scalar operator O_l^0.[6,7] The obtained eigenvectors are related to the orthonormalized quadrupole-phonon wave functions, often used in nuclear structure calculations. The O_l^0 eigenvalue can be interpreted as a fifth label for these states, which are also specified by the phonon number N, the seniority quantum number v, the total angular momentum l and its projection m. The method developed for extracting these eigenvalues and eigenvectors is quite involved. It is based upon a tree generating mechanism. This means that for a fixed v-value the O_l^0 eigenvalue of one of the existing $|v,l,m\rangle$ states cannot be uniquely deduced if all eigenvalues belonging to all the other existing $|v,l,m\rangle$ states have not been calculated. Having derived the relations between the scalar product operators of the P_l^k and O_l^k type for the R(7) group,[2,3] we established that the previously used tree generating mechanism does not generally lead in that case to the P_l^0 and O_l^0 eigenvalues. In order to simplify the determination of the O_l^0 eigenvalues and the corresponding eigenvectors for the quadrupole-phonon states and to create a possibility of deducing the P_l^0 and O_l^0 eigenvalues and eigenvectors in the octupole-phonon case, the study of quadratic product operators of the type $O_{l+k}^{\ j}O_l^{+k}$ ($-3\leqslant j,k\leqslant +3$, and $0<|j+k|\leqslant 6$) and $P_{l+k}^{\ j}P_l^{+k}$ ($-5\leqslant j,k\leqslant +5$ and $0<|j+k|\leqslant 10$), which have no R(3) scalar character, is of great importance. In this paper we shall restrict ourselves to the investigation of the nonscalar R(3) product operators of the form $O_{l+k}^{\ j}O_l^{+k}$ in the quadrupole- as well as in the octupole-phonon case.

2. HERMITICITY PROPERTIES

As already mentioned by Hughes and Yadegar[5] and by ourselves (Ref.[1], to be referred to as I), the $O_l^{\pm k}$ are related by hermiticity

$$\langle l,a_l,m|(O_l^{+k})^\dagger|l+k,b_{l+k},m\rangle = \beta_{kl}\langle l,a_l,m|O_{l+k}^{-k}|l+k,b_{l+k},m\rangle, \tag{2.1}$$

with $\beta_{kl} = (2l+1)/(2l+2k+1)$. Following Hughes,[4] the eigenvectors of the angular momentum operator L^2 and its projection l_0, upon which the $O_l^{\pm k}$ acts, are denoted by the kets $|l,a_l,m\rangle$, where a_l represents the evential labels necessary for a unique classification of the state.

As it was the case for the scalar R(3) quadratic product operators there also exist relations connecting the matrix elements of nonscalar R(3) product operators. The proofs of these relations are based on (2.1) and are completely similar to the ones given by Hughes[4] for the scalar case. Therefore we shall only state the results

$$\langle l+k-j,c_{l+k-j},m|O_{l+k}^{\ j}O_l^{+k}|l,a_l,m\rangle = \frac{1}{\beta_{j,l+k-j}}\sum_{b_{l+k}}\langle l+k,b_{l+k},m|O_{l+k-j}^{+j}|l+k-j,c_{l+k-j},m\rangle' \times\langle l+k,b_{l+k},m|O_l^{+k}|l,a_l,m\rangle, \tag{2.2}$$

and

$$\sum_{a_l,c_{l-k+j}}\langle l-k+j,c_{l-k+j},m|O_{l-k}^{+j}O_l^{-k}|l,a_l,m\rangle = \beta_{j-k,l}\sum_{a_l,c_{l-k+j}}\langle l,a_l,m|O_{l-k}^{+k}O_{l-k+j}^{-j}|l-k+j,c_{l-k+j}\rangle^*. \tag{2.3}$$

In the special case $j = k$ [the scalar R(3) situation] and choosing $c_l \equiv a_l$, (2.2) and (2.3) respectively reduce to (I.4.1),(I.4.3) and (I.4.4),(1.4.5).

3. THE NONSCALAR R(3) PRODUCT OPERATORS AND THEIR MUTUAL RELATIONS

The quadratic operator $O_{l+k}^{\ j}O_l^{+k}$ ($-3\leqslant j,k\leqslant 3$ and

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$0 \leqslant |j+k| \leqslant 6$) shifts the l value of the state upon which it acts by $(k+j)$. With the available shift operators (I.2.1)–(1.2.5), which contain the q_μ to first order only, one can construct seven product operators with $s = j + k = 0$, six with $s = -1$, five with $s = -2$, four with $s = -3$, three with $s = -4$, two with $s = -5$, and one with $s = -6$. For $s = 0$ (the scalar case) we have shown in I and Ref. 2 (hereafter denoted as V) that four independent relations exist between these scalar R(3) product operators. It has to be noted that these expressions are only valid when they act to the right upon states with angular momentum projection $m = 0$. It has been remarked that this seemingly drastic condition does not seriously detract from the generality of the presented calculations. Therefore we shall work here also within this same convention.

The considered quadratic product operators consist of terms composed of two q_μ and six or less l_i operators. In order to obtain relations between them it is clear that once again all product operators should be brought into a standard form. The procedure to reach that form has been fully discussed in I. It has to be remarked in advance that on account of the commuting properties of the q generators (see I and V), operators where q generators as well as p generators (for the octupole case) appear linearly, can emerge in relations between quadratic products of the shift operators O_l^k. It is easy to predict that in relations between expressions of the form $O_{l+k}^{+j} O_l^{+k}$, these operators, linear in q_μ and p_μ, will be O_l^{j+k} and P_l^{j+k} themselves, if they are defined. By straightforward calculation we have arrived at the following final results for the cases where $k + j < 0$.

$$\frac{(l+2)^2(2l+3)(2l+5)}{l} O_{l-1}^0 O_l^{-1} - \frac{(l+2)(l+6)(2l+1)(2l+5)}{l} O_1^{-1} O_l^0$$
$$- \frac{3(2l+3)(2l+7)}{(l+1)^2} O_{l+1}^{-2} O_l^{+1} - \frac{3(2l+1)}{(l+1)^2(l+2)^2} O_{l+2}^{-3} O_l^{+2}$$
$$= A_\lambda (l+1)(l+2)^2(2l+1)(2l+3)(2l+5) O_l^{-1} + \frac{(\lambda-2)}{\sqrt{3}} (l+1)(l+2)(2l+1)(2l+3) P_l^{-1}, \tag{3.1}$$

$$\frac{(l-2)(l-6)(2l-1)(2l-5)}{l} O_{l-1}^0 O_l^{-1} - \frac{(l-2)^2(2l-3)(2l-5)}{l} O_l^{-1} O_l^0$$
$$- \frac{3(2l-3)(2l-7)}{(l-1)^2} O_{l-2}^{+1} O_l^{-2} + \frac{3(2l-1)}{(l-1)^2(l-2)^2} O_{l-3}^{+2} O_l^{-3}$$
$$= A_\lambda (l-1)(l-2)^2(2l-1)(2l-3)(2l-5) O_l^{-1} + \frac{(\lambda-2)}{\sqrt{3}} (l-1)(l-2)(2l-1)(2l-3) P_l^{-1}, \tag{3.2}$$

$$\frac{(l+1)(2l-1)(4l^2-8l-41)}{l} O_{l-1}^0 O_l^{-1} - \frac{(l-1)(2l+1)(4l^2+8l-41)}{l} O_l^{-1} O_l^0$$
$$- \frac{3(l-1)(2l-1)(2l-3)}{l(l+1)^2} O_{l+1}^{-2} O_l^{+1} - \frac{3(l+1)(2l+1)(2l+3)}{l(l-1)^2} O_{l-2}^{+1} O_l^{-2}$$
$$= A_\lambda (l+1)(l-1)(2l+1)(2l-1)(4l^2+11) O_l^{-1} + \frac{2(\lambda-2)}{\sqrt{3}} (l+1)(l-1)(2l+1)(2l-1) P_l^{-1}, \tag{3.3}$$

$$\frac{(l+1)(l+2)(2l+1)(2l+3)}{l(l-1)} O_{l-2}^0 O_l^{-2} - \frac{(2l+1)(2l^2-l-30)}{l} O_l^{-2} O_l^0$$
$$- \frac{3(l-2)(2l-1)}{l(l+1)^2} O_{l+1}^{-3} O_l^{+1} - 15 \frac{(l+1)(l+2)(2l-1)}{l(l-1)} O_{l-1}^{-1} O_l^{-1}$$
$$= A_\lambda (l+1)(l+2)(2l-1)(2l+1)(2l+3) O_l^{-2} - \frac{2(\lambda-2)}{\sqrt{3}} (l+1)(2l-1)(2l+1) P_l^{-2}, \tag{3.4}$$

$$\frac{6(l+1)(l+2)}{l} O_{l-2}^0 O_l^{-2} + \frac{6(l-2)(l-3)}{(l-1)} O_l^{-2} O_l^0$$
$$- \frac{(l-2)^2(l-3)}{l(l+1)^2} O_{l+1}^{-3} O_l^{+1} + \frac{(l+1)^2(l+2)}{(l-1)(l-2)^2} O_{l-3}^{+1} O_l^{-3}$$
$$= 4A_\lambda (l-2)(l-3)(l+1)(l+2)(2l-1) O_l^{-2} + \frac{2(\lambda-2)}{\sqrt{3}} (l-2)(l+1)(2l-1) P_l^{-2}, \tag{3.5}$$

$$l(2l-1) O_{l-3}^0 O_l^{-3} - (l-2)(2l-3) O_l^{-3} O_l^0 + 3(l-2)(2l-1) O_{l-1}^{-2} O_l^{-1} - 3l(2l-3) O_{l-2}^{-1} O_l^{-2}$$
$$= -3A_\lambda l(l-1)(l-2)(2l-1)(2l-3) O_l^{-3}, \tag{3.6}$$

$$(l-2)(l-4) O_{l-1}^{-3} O_l^{-1} - (l-1)(l+1) O_{l-3}^{-1} O_l^{-3} + 3(2l-3) O_{l-2}^{-2} O_l^{-2}$$
$$= \frac{(\lambda-2)}{\sqrt{3}} (l-1)(l-2)(2l-3) P_l^{-4}, \tag{3.7}$$

$$O_{l-2}^{-3} O_l^{-2} - O_{l-3}^{-2} O_l^{-3} = -\frac{(\lambda-2)}{\sqrt{3}} (l-2) P_l^{-5}. \tag{3.8}$$

Once more we like to insist on the fact that these right relations are only valid when they are acting to the right upon $m = 0$ states. They can be used either for the quadrupole phonons ($\lambda = 2$) as well as for the octupole phonons ($\lambda = 3$). In these cases the A_λ parameter respectively takes the following numerical values $A_2 = -\sqrt{2}/5, A_3 = \sqrt{2}/\sqrt{15}$. In order to show that the P_l^k operators are only playing a role for octupole phonons, we have introduced the factor $(\lambda - 2)$. As long as four or more product operators $O_{l+k}^{+j} O_l^{+k}$ for a fixed $(k + j)$ value exist, it occurs again that at least four of these operators are needed to build up the mentioned relations. The same feature has been observed for the scalar R(3) case (see I and V). Furthermore one can note that in (3.6) no P_l^{-3} term occurs. This is due to the fact that all terms where the p_μ factors linearly appear accidentally become zero for this special relation. Using the fact that O_l^{+k} and O_l^{-k} go over into each other on replacing l by $-(l + 1)$, eight other equations can be easily derived from (3.1)–(3.8). The reader can easily perform this transformation himself if such relations are of importance.

4. CONCLUSIONS

We have demonstrated how the results derived in I and V between scalar R(3) objects in the context of the multipole labeling problem, can be extended to the case of the nonscalar R (3) operator products. The detailed relations derived in this paper, although rather technical, will prove to be extremely useful in some following papers where eigenvalues of O_l^0 will be derived for the quadrupole as well as for the octupole phonons. It is evident that analogous relations can be constructed of the type $P_{l+k}^{+j} P_l^{+k}$ ($-5 \leqslant j,k \leqslant +5$ and $0 < |j + k| T \leqslant 10$). This will be reported in a subsequent paper. By multiplying the right side of (3.1)–(3.3) by O_{l-l}^{+1}, (3.4), (3.5) by O_{l-2}^{+2}, and (3.6) by O_{l-3}^{+3}, respectively, one obtains relations between scalar R(3) triple product operators and scalar R(3) quadratic product operators. By an appropriate substitution it might be possible to derive a relation between such triple product operators and the other available invariants, such as O_l^0, L^2, V^*. By this remark, the conjecture that it was not possible to derive explicit expressions for such products in practice, made in I, is nullified.

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Shift operator techniques for the classification of multipole-phonon states. VII. Self-consistent single step algorithm for R(5) O_l^0 eigenstate and eigenvalue determination

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A previously derived set of quadratic relations in the R(5) shift operators O_l^k ($|k| \leqslant 3$), is shown to be in such a way complete, that any O_l^0 eigenvector and corresponding eigenvalue can be unambiguously obtained in a step by step calculation which starts at the highest angular momentum state. Such a calculation strictly follows the pattern of an algorithm, which unlike the tree generating mechanism, has unlimited applicability. Previous knowledge of the existence and of the degeneracy of a state not being required the algorithm itself accounts for the l multiplicity of states and is therefore called self-consistent.

1. INTRODUCTION

In a set of previous papers[1-6] (to be referred to as I to VI), part of the quadrupole eigenvalue spectrum[2] of the R(3) scalar shift operator[1] O_l^0 has been derived by means of the relations[1] existing between R(3) scalar product operators $O_{l+k}^{-k} O_l^{+k}$ ($|k| \leqslant 3$), the seniority operator V^*, and the shift operator O_l^0. In the preceding paper[6] we constructed additional relations, also quadratic in the shift operators O_l^k ($|k| \leqslant 3$), but involving products of the form $O_{l+k}^j O_l^k$, where $-3 \leqslant j, k \leqslant 3$ and $0 < |j+k| \leqslant 5$.

The major concern of the present paper is to illustrate, by taking the R(5) quadrupole case as a test case, the main advantages of including the latter set of relations into eigenvalue calculations. At the same time we shall develop a straightforward calculation technique, which on account of its extended validity, can be applied to the octupole case[4,5] as well.

The most important feature of the present technique is that we can completely abandon the tree generating mechanism expounded in II, which for the unambiguous determination of a particular eigenvalue, $\alpha_{v,l}$ say, necessitated the calculation of all the eigenvalues in the set $\{\alpha_{v,l} | l = 2v, 2v-2, \ldots, 2 \text{ or } 0\}$. With the new method, once $\alpha_{v,2v}$ corresponding to the maximum angular momentum state $|v, 2v\rangle$ is known, all eigenvalues associated to states with the same seniority v are consecutively generated in a single step procedure. Hence, we shall be able to prove that the expressions for the matrix elements of scalar product operators and for the O_l^0 eigenvalues deduced in II for $v \leqslant 7$, remain valid for all $v > 7$. Moreover, we also shall derive new formulas which by no means could be obtained with tree generation, more precisely formulas producing the $\alpha_{v,2v-6}$ and $\alpha_{v,2v-7}$ eigenvalues for all possible v, and a similar one leading immediately to the eigenvalues $\alpha_{v,6}$ for $v = 3k$ and $k > 1$.

Finally we note that the eigenvalue computations and hence also the labeling of the states were carried out in II independently from the explicit construction of the eigenstates in III. With the present technique both problems will be solved simultaneously. Moreover, it is not even necessary to know in advance if states exist or if states are degenerated or not. Indeed, it shall turn out that the l-multiplicity of states follows naturally from the construction of these states. In this sense the new formalism is not only complete but also self-consistent.

2. THE HIGH ANGULAR MOMENTUM STATES AND THEIR EIGENVALUES

In II we showed how the O_{2v}^0 eigenvalue $\alpha_{v,2v}$ of the maximum angular momentum state $|v, 2v\rangle$ with seniority v is found in an unambiguous way by combining Eqs. (I.3.2) and (I.3.5), both acting on the $|v, 2v\rangle$ state. However, in the proof it was understood that $|v, 2v-1\rangle$ states did not exist and hence that the matrix element $\langle v, 2v | O_{2v-1}^{+1} O_{2v}^{-1} | v, 2v\rangle$ was zero.

As explained in the introductory section, we like to investigate here whether the quadratic relations in the shift operators themselves can account for the nonexistence of any $|v, 2v-1\rangle$ state. Consequently, let us assume that there is a $|v, 2v-1\rangle$ state, which is then obviously defined by means of the relation

$$O_{2v}^{-1} |v, 2v\rangle = a |v, 2v-1\rangle, \tag{2.1}$$

where a is a factor which should be fixed by the condition that $|v, 2v-1\rangle$ is a normalized state. Following (III.2.9) and (III.2.10) (in the latter formula a square root symbol has been erroneously omitted) a is given upon a phase factor by

$$|a| = \left(\frac{4v+1}{4v-1} \langle v, 2v | O_{2v-1}^{+1} O_{2v}^{-1} | v, 2v \rangle \right)^{1/2}. \tag{2.2}$$

If we let Eq. (I.3.2) act on the $|v, 2v\rangle$ state, we obtain the quadratic equation (II.2.1) in $\alpha_{v,2v}$. On the other hand, Eq. (I.3.5) acting on the $|v, 2v\rangle$ state now also involves the matrix element occurring in (2.2) and reduces after a few calculations to

$$\begin{aligned}(16v^2 + 57v + 45)\,\alpha_{v,2v}^2 - \tfrac{2}{15}\sqrt{2}v(2v+1)(4v+3)(16v^3 &+ 68v^2 + 87v + 45)\,\alpha_{v,2v} \\ = \tfrac{8}{75}v^2(v+1)(2v+1)^2(4v+3)^2(32v^3 &+ 151v^2 + 219v + 90) - \frac{(v+1)(4v+3)(4v^2+14v+15)}{4v^2(4v+1)} \\ &\times \langle v, 2v | O_{2v-1}^{+1} O_{2v}^{-1} | v, 2v \rangle.\end{aligned} \tag{2.3}$$

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From Eq. (II.2.1) it follows that $\alpha_{v,2v}$ can either be expressed as

$$\alpha_{v,2v} = \tfrac{2}{5}\sqrt{2}v(v+1)(2v+1)(4v+3), \tag{2.4}$$

or as

$$\alpha_{v,2v} = -\tfrac{2}{5}\sqrt{2}(v+1)^2(2v+1)(4v+3). \tag{2.5}$$

Substituting the result (2.4) into (2.3) the matrix element $\langle v, 2v|O^{+1}_{2v-1}O^{-1}_{2v}|v, 2v\rangle$ is found to become zero, whereas the substitution of (2.5) into that equation leads to the following expression for the same matrix element

$$\langle v, 2v|O^{+1}_{2v-1}O^{-1}_{2v}|v, 2v\rangle = -\tfrac{32}{75}v^2(2v+1)^3(v+3)(4v+1)(4v+3)^2.$$

In view of the property (I.4.5) a matrix element of the kind $\langle v, 2v|O^{+j}_{2v-j}O^{-j}_{2v}|v, 2v\rangle$ with $j \leqslant 3$ is necessarily a non-negative quantity. Therefore, (2.5) cannot be the true expression for $\alpha_{v,2v}$ and we are left with the solution (2.4) which leads to the vanishing matrix element $\langle v, 2v|O^{+1}_{2v-1}O^{-1}_{2v}|v, 2v\rangle$, hence by (2.2) also to zero a value and finally by (2.1) to the nonexistence of any $|v, 2v-1\rangle$ state.

The unambiguous determination of the $\alpha_{v,2v-2}$ eigenvalues is the first example which illustrates the advantages connected with the use of the relations between the nonscalar R(3) product operators derived in VI. Indeed, if a $|v, 2v-2\rangle$ state exists, necessarily it is implicitly defined as

$$O^{-2}_{2v}|v, 2v\rangle = a|v, 2v-2\rangle, \tag{2.6}$$

where a is again a normalization factor. Also

$$|a| = \left(\frac{(4v+1)}{(4v-3)}\langle v, 2v|O^{+2}_{2v-2}O^{-2}_{2v}|v, 2v\rangle\right)^{1/2}. \tag{2.7}$$

Next, letting Eq. (VI.3.4) act on the $|v, 2v\rangle$ state we obtain after some cancellations

$$\begin{aligned}&\frac{(v+1)(2v+1)(4v+3)}{v(2v-1)}O^0_{2v-2}[O^{-2}_{2v}|v, 2v\rangle] \\ &\quad - \frac{(4v^2-v-15)}{v}\alpha_{v,2v}[O^{-2}_{2v}|v, 2v\rangle] \\ &= -\frac{2^2\sqrt{2}}{5}(v+1)(2v+1)(4v-1)(4v+3) \\ &\quad \times [O^{-2}_{2v}|v, 2v\rangle].\end{aligned}$$

Substituting in here relation (2.6) and the expression for $\alpha_{v,2v}$ given in (2.4), one immediately deduces that

$$\begin{aligned}\alpha_{v,2v-2} &= \langle v, 2v-2|O^0_{2v-2}|v, 2v-2\rangle \\ &= \tfrac{2}{5}\sqrt{2}v(2v-1)(4v^2-5v-14),\end{aligned} \tag{2.8}$$

which corresponds to formula (II.4.2), but which is now proven to be valid for all $v > 1$.

There remains the problem of finding the matrix element $\langle v, 2v|O^{+2}_{2v-2}O^{-2}_{2v}|v, 2v\rangle$. To this aim we can simply use (as we did before in II) the scalar product operator relation (I.3.3) acting on the $|v, 2v\rangle$ state. All terms therein being known, except for the desired matrix element which occurs linearly, it is straightforward to retrieve the result listed in (II.4.19), i.e.,

$$\langle v, 2v|O^{+2}_{2v-2}O^{-2}_{2v}|v, 2v\rangle = \frac{2^7}{3}v^4(v-1)(2v+1)^2(2v-1)^3 \times(4v+1). \tag{2.9}$$

From (2.9), and taking into account (2.6) and (2.7), we can conclude that

$$\begin{aligned}O^{-2}_{2v}|v, 2v\rangle &= 2^3v^2(2v+1)(2v-1)(4v+1) \\ &\quad \times[2(v-1)(2v-1)/3(4v-3)]^{1/2}|v, 2v-2\rangle,\end{aligned} \tag{2.10}$$

where we can have selected the positive square root.

3. THE SYSTEMATIC LOWERING OF THE ANGULAR MOMENTUM

As a next step, let us consider the construction of $|v, 2v-3\rangle$ states. In contrast to what occurred before, we have now two possibilities to define a $|v, 2v-3\rangle$ state by means of an l-lowering shift operator action on a state with higher angular momentum, namely, $O^{-3}_{2v}|v, 2v\rangle$ and $O^{-1}_{2v-2}|v, 2v-2\rangle$. Consequently we shall assume two independent orthonormal $|v, 2v-3\rangle$ states, denoted by $|v, 2v-3, (1)\rangle$ and $|v, 2v-3, (2)\rangle$ exist. Hence, we can set

$$O^{-3}_{2v}|v, 2v\rangle = a_1|v, 2v-3, (1)\rangle + a_2|v, 2v-3, (2)\rangle, \tag{3.1}$$

$$O^{-1}_{2v-2}|v, 2v-2\rangle = b_1|v, 2v-3, (1)\rangle + b_2|v, 2v-3, (2)\rangle, \tag{3.2}$$

where a_1, a_2, b_1, b_2 are yet unknown coefficients which without loss of generality we can assume to be real. According to the hermiticity property (VI.2.1), Eq. (3.1) can be rewritten as

$$\begin{aligned}\beta_{-3,2v}\langle v, 2v|O^{+3}_{2v-3} &= \langle v, 2v-3, (1)|a_1 \\ &\quad + \langle v, 2v-3, (2)|a_2,\end{aligned}$$

whereafter multiplication by (3.1) yields on account of orthonormality

$$a_1^2 + a_2^2 = \beta_{-3,2v}\langle v, 2v|O^{+3}_{2v-3}O^{-3}_{2v}|v, 2v\rangle. \tag{3.3}$$

Similarly

$$b_1^2 + b_2^2 = \beta_{-1,2v-2}\langle v, 2v-2|O^{+1}_{2v-3}O^{-1}_{2v-2}|v, 2v-2\rangle. \tag{3.4}$$

The relations (3.3) and (3.4) are the immediate generalizations of a singular state relation such as (2.2) or (2.7). The matrix elements of the scalar product operators on the right-hand sides of (3.3) and (3.4) can be unambiguously determined by use of the scalar relations (I.3.4) and (I.3.5) acting on the $|v, 2v\rangle$ and the $|v, 2v-2\rangle$ state, respectively, and are given in (II.4.19). It follows with the help of (2.9) that

$$\begin{aligned}a_1^2 + a_2^2 &= 2^9v^4(v-1)^3(v-2)(2v-1)^2 \\ &\quad \times(4v+1)^2(4v-1)(4v-3)/(4v-5),\end{aligned} \tag{3.5}$$

$$\begin{aligned}b_1^2 + b_2^2 &= \frac{2^5}{3}(v-1)^2(v-2)(2v+1)^2 \\ &\quad \times(2v-1)(4v-1)(4v-3)^2/(4v-5).\end{aligned} \tag{3.6}$$

In accordance with the notations of I–VI we set

$$O^0_{2v-3}|v, 2v-3, (i)\rangle = \alpha_{v,2v-3}(i)|v, 2v-3, (i)\rangle, \quad (i \doteq 1, 2). \tag{3.7}$$

If we then let Eq. (VI.3.6) act on the $|v, 2v\rangle$ state, and if we substitute therein the expression for $\alpha_{v,2v}$ and also make use

of (3.1), (3.2), and (2.10), we obtain on account of the orthogonality of the $|v, 2v-3, (i)\rangle$ states and after some rearrangements the following equations between the unknowns a_i and b_i $(i=1, 2)$

$$2\Big[(4v-1)\alpha_{v,2v-3}(i) - \tfrac{2}{5}\sqrt{2}(v-1)(4v-3)(8v^3+42v^2 - 5v+6)\,]a_i - 2^4 3v^2(2v+1)(2v-1)(4v+1) \times[2(v-1)(2v-1)(4v-3)/3\,]^{1/2} b_i = 0, \quad (i=1,2). \tag{3.8}$$

In the same way, Eq. (VI.3.1) acting on the $|v, 2v-2\rangle$ state leads to the equations

$$2\cdot 3\cdot(v-1)(2v+1)(4v-3)\,[2(v-1)(2v-1) \times(4v-3)/3\,]^{1/2} a_i - 2v^2(2v-1)(4v+1)\,[(4v-1)\alpha_{v,2v-3}(i) - \tfrac{2}{5}\sqrt{2}(2v-1)(4v-3)(4v^3-v^2-19v-29)\,\Big] b_i = 0, \quad (i=1,2), \tag{3.9}$$

where we have also used the property

$$\langle v, 2v | O^{+2}_{2v-2} | v, 2v-2\rangle = [\beta_{2,2v-2}\langle v, 2v-2 | O^{-2}_{2v} O^{+2}_{2v-2} | v, 2v-2\rangle]^{1/2} = [\beta_{2,2v-2}\langle v, 2v | O^{+2}_{2v-2} O^{-2}_{2v} | v, 2v\rangle]^{1/2},$$

which is based on the fact that both $|v, 2v\rangle$ and $|v, 2v-2\rangle$ are nondegenerated states.

The four linear homogeneous equations (3.8), (3.9) lead to nonzero a_i and b_i if $\alpha_{v,2v-3}(1)$ and $\alpha_{v,2v-3}(2)$ are the two solutions of the quadratic equation

$$(4v-1)x^2 - \tfrac{2}{5}\sqrt{2}(4v-3)(16v^4+28v^3-84v^2-28v+23) \times x + \frac{2^3}{5^2}(v-1)(2v-1)(4v-3)^2(8v^5+42v^4 - 43v^3-411v^2-385v+24) = 0.$$

Hence, solving this equation we can set

$$\alpha_{v,2v-3}(1) = \tfrac{2}{5}\sqrt{2}(4v-3)(2v^3-v^2-17v+1), \tag{3.10}$$

$$\alpha_{v,2v-3}(2) = \tfrac{1}{5}\sqrt{2}(4v-3)(8v^4+34v^3-17v^2-49v+24)/(4v-1). \tag{3.11}$$

Substitution of the expressions (3.10), (3.11) in (3.8) and (3.9) yields the relations,

$$b_1 = -(2v+1)(4v-3)/\{2^2v^2(4v+1) \times[3(v-1)(2v-1)(4v-3)\,]^{1/2}\} a_1, \tag{3.12}$$

$$b_2 = \sqrt{3}(v-1)^2(4v-3)/\{2v^2(2v+1)(2v-1) \times(4v+1)\,]\times[(v-1)(2v-1)(4v-3)\,]^{1/2}\} a_2, \tag{3.13}$$

which by means of Eq. (3.6) allows us to find, in addition to Eq. (3.5), a second equation in the unknowns a_1^2 and a_2^2. The two equations have a unique solution which reads

$$a_1^2 = 2^9 v^4(v-1)^3(v-2)(2v-1)^2(4v+1)^2(4v-1)(4v-3)/(4v-5),$$

$$a_2^2 = 0. \tag{3.14}$$

This solution clearly demonstrates that only the state $|v, 2v-3, (1)\rangle$ is reached and has to be retained, whereas $|v, 2v-3, (2)\rangle$ can be abandoned. Consequently it is proved that there exists only a unique $|v, 2v-3\rangle$ state, or otherwise stated $|v, 2v-3\rangle$ is nondegenerated. Choosing a_1 to be the positive square root of the right-hand side of (3.14) the final results can be resumed in

$$O^{-3}_{2v}|v, 2v\rangle = 2^4 v^2(v-1)(2v-1)(4v+1) \times[2(v-1)(v-2)(4v-1)(4v-3) /(4v-5)\,]^{1/2}|v, 2v-3\rangle,$$

$$O^{-1}_{2v-2}|v, 2v-2\rangle = -2^2(v-1)(2v+1)(4v-3) \times[2(v-2)(2v-1)(4v-1) /3(4v-5)\,]^{1/2}|v, 2v-3\rangle,$$

$$\alpha_{v,2v-3} = \tfrac{2}{5}\sqrt{2}(4v-3)(2v^3-v^2-17v+1) \quad (v>2). \tag{3.15}$$

These formulas confirm the corresponding ones derived in II for $v<7$.

The application of a reasoning similar to the one above [and more precisely the use of the relations (VI.3.1)–(VI.3.8)] for the construction of $|v, 2v-4\rangle$ states, turns out to lead almost immediately to the well-known property of nondegeneracy for these states. Indeed, having again two possibilities to generate $|v, 2v-4\rangle$ states by means of l-lowering shift operators, namely $O^{-2}_{2v-2}|v, 2v-2\rangle$ and $O^{-1}_{2v-3}|v, 2v-3\rangle$ one should at first introduce two orthonormal $|v, 2v-4\rangle$ states. However, if we let Eq. (VI.3.7) act on the $|v, 2v\rangle$ state we obtain after substitution of $O^{-2}_{2v}|v, 2v\rangle$ and $O^{-3}_{2v}|v, 2v\rangle$ by their expressions given in (2.10) and (3.15), respectively, the relation

$$2(v-1)\,[(v-2)(2v-1)(4v-1)\,]^{1/2} O^{-1}_{2v-3}|v, 2v-3\rangle = [3(4v-5)\,]^{1/2} O^{-2}_{2v-2}|v, 2v-2\rangle. \tag{3.16}$$

Hence, $O^{-1}_{2v-3}|v, 2v-3\rangle$ and $O^{-2}_{2v-2}|v, 2v-2\rangle$ not being independent, only one $|v, 2v-4\rangle$ state exists and has to be further taken into account. Since the relation (I.3.3) alone is sufficient to derive unambiguously the matrix element $\langle v, 2v-2|O^{+2}_{2v-4} O^{-2}_{2v-2}|v, 2v-2\rangle$ of which the expression is given in (II.4.19), it is immediately proven by choosing once more the positive square root, that

$$O^{-2}_{2v-2}|v, 2v-2\rangle = 2^4(v-1)(2v-1)(2v-3) \times[(v-1)(v-2)(v-3)(2v+1)(4v-1) \times(4v-3)/3(4v-7)\,]^{1/2}|v, 2v-4\rangle. \tag{3.17}$$

From (3.16) it also follows that

$$O^{-1}_{2v-3}|v, 2v-3\rangle = 2^3(2v-3)\,[(v-1)(v-3)(2v+1)(2v-1)(4v-3) \times(4v-5)/(4v-7)\,]^{1/2}|v, 2v-4\rangle. \tag{3.18}$$

It has to be noted that, apart from the sign, (3.18) can also be obtained by substituting in the relation $O^{-1}_{2v-3}|v, 2v-3\rangle = [\beta_{-1,2v-3}\langle v, 2v-3|O^{+1}_{2v-4} O^{-1}_{2v-3}|v, 2v-3\rangle\,]^{1/2}$ the matrix element by its expression expounded in (II.4.19). As for calculating the eigenvalue $\alpha_{v,2v-4}$, we can, for example, use Eq. (VI.3.4) acting on the $|v, 2v-2\rangle$ state, to find with the help of (3.15), (3.17), and (3.18) that

$$\alpha_{v,2v-4} = \tfrac{2}{5}\sqrt{2}(v-1)(8v^3-38v^2-v-60), \quad (v>3). \tag{3.19}$$

This is exactly what we found previously in (II.4.4) for $v\leqslant 7$.

By treating the $|v, 2v-5\rangle$ states, for the first time it happens that there are three different ways to generate these states, i.e., $O^{-3}_{2v-2}|v, 2v-2\rangle$, $O^{-2}_{2v-3}|v, 2v-3\rangle$, and $O^{-1}_{2v-4}|v, 2v-4\rangle$. Consequently, we have to begin with the assumption that three orthonormalized $|v, 2v-5\rangle$ states exist. However, exactly in the same way as in the case of the $|v, 2v-4\rangle$ states, now equation (VI.3.8) provides us immediately with a relationship between $O^{-3}_{2v-2}|v, 2v-2\rangle$ and $O^{-2}_{2v-3}|v, 2v-3\rangle$, a fact which at once reduces the maximal number of independent $|v, 2v-5\rangle$ states already to two. From that point on, the calculations ressemble those related to the $|v, 2v-3\rangle$ state construction and eigenvalue calculation. Again it turns out at the end that only one $|v, 2v-5\rangle$ state must be witheld. The results of the calculations can be resumed as follows:

$$O^{-3}_{2v-2}|v, 2v-2\rangle = 2^4(v-1)(v-2)(2v-3)(4v-3)\ [2(v-1)(v-2)(v-3) \times(v-4)(4v-1)(4v-5)/(4v-9)\ ]^{1/2}|v, 2v-5\rangle,$$

$$O^{-2}_{2v-3}|v, 2v-3\rangle = 2^3(v-2)(2v+1)(2v-3)(4v-5)\ [2(v-1)(v-3)(v-4) \times(2v-1)/3(4v-9)\ ]^{1/2}|v, 2v-5\rangle,$$

$$O^{-1}_{2v-4}|v, 2v-4\rangle = -2^3(v-2)(2v-1)\ [(v-4)(2v+1)(4v-3)(4v-5) \times(4v-7)/3(4v-9)\ ]^{1/2}|v, 2v-5\rangle,$$

and

$$\alpha_{v,2v-5} = \tfrac{2}{5}\sqrt{2}(8v^4-42v^3-77v^2+258v-150) \quad (v>4). \tag{3.20}$$

So far we have invoked numerous quadratic shift operator relations, to prove that the formulas (II.4.1)–(II.4.5) and (II.4.19) remain valid for all seniorities. Thus, although the l multiplicity of eigenstates could any time be rigorously deduced from the relations, only well-known results have been retrieved yet. Therefore we shall proceed here with the treatment of the $|v, 2v-6\rangle$ states, a case which is impossible to handle with the tree generating mechanism for general v number.

Again there are three possibilities to generate the $|v, 2v-6\rangle$ states, but Eq. (VI.3.7) provides us already with a first relation between $O^{-3}_{2v-3}|v, 2v-3\rangle$, $O^{-2}_{2v-4}|v, 2v-4\rangle$, and $O^{-1}_{2v-5}|v, 2v-5\rangle$. Consequently we can put

$$O^{-3}_{2v-3}|v, 2v-3\rangle = a_1|v, 2v-6, (1)\rangle + a_2|v, 2v-6, (2)\rangle, \tag{3.21}$$

$$O^{-2}_{2v-4}|v, 2v-4\rangle = b_1|v, 2v-6, (1)\rangle + b_2|v, 2v-6, (2)\rangle, \tag{3.22}$$

$$O^{-1}_{2v-5}|v, 2v-5\rangle = c_1|v, 2v-6, (1)\rangle + c_2|v, 2v-6, (2)\rangle, \tag{3.23}$$

whereas, since $|v, 2v-6, (1)\rangle$ and $|v, 2v-6, (2)\rangle$ are assumed to be normalized and orthogonal to each other, Eq. (VI.3.7) can be written in terms of the unknowns a_i, b_i, and c_i as

$$\begin{aligned}&(v-2)(v-3)(2v+1)(4v-3)\ [2(2v-1)/3(4v-5)\ ]^{1/2}a_i \\ &\quad -3(2v-1)(2v-3)(4v-7) \\ &\quad \times[(v-1)(v-3)(2v+1)(4v-3)/3(4v-7)\ ]b_i \\ &\quad +(v-2)(2v-1)(2v-3)^2(4v-3) \\ &\quad \times[2(v-1)(v-3)(v-4)(4v-5)/(4v-9)\ ]^{1/2}c_i \\ &\quad =0 \quad (i=1,2).\end{aligned} \tag{3.24}$$

Furthermore, it is easily demonstrated that

$$a_1^2+a_2^2=\beta_{-3,2v-3}\langle v, 2v-3|O^{+3}_{2v-6}O^{-3}_{2v-3}|v, 2v-3\rangle, \tag{3.25}$$

$$b_1^2+b_2^2=\beta_{-2,2v-4}\langle v, 2v-4|O^{+2}_{2v-6}O^{-2}_{2v-4}|v, 2v-4\rangle, \tag{3.26}$$

$$c_1^2+c_2^2=\beta_{-1,2v-5}\langle v, 2v-5|O^{+1}_{2v-6}O^{-1}_{2v-5}|v, 2v-5\rangle, \tag{3.27}$$

if a_i, b_i, c_i $(i=1, 2)$ are real quantities. The matrix elements in (3.25)–(3.27) can be unambiguously determined by the use of the scalar product operator relations (I.3.2)–(I.3.5). After straightforward but lengthy calculations, one finds

$$\begin{aligned}&\langle v, 2v-3|O^{+3}_{2v-6}O^{-3}_{2v-3}|v, 2v-3\rangle \\ &\quad =2^5(v-1)(v-2)^2(2v-1)(2v-3)^3(2v-5)^2 \\ &\quad \times(128v^4-1376v^3+5608v^2-10042v+6465), \\ &\langle v, 2v-4|O^{+2}_{2v-6}O^{-2}_{2v-4}|v, 2v-4\rangle \\ &\quad =2^7(v-2)^2(2v-3)(2v-5)^2(4v-3) \\ &\quad \times(4v^5-44v^4+167v^3-269v^2+228v-110), \\ &\langle v, 2v-5|O^{+1}_{2v-6}O^{-1}_{2v-5}|v, 2v-5\rangle \\ &\quad =\frac{2^5}{3}(2v+1)(2v-3)(2v-5)^2 \\ &\quad \times(16v^4-72v^3-155v^2+693v-536).\end{aligned} \tag{3.28}$$

Next, letting Eq. (VI.3.6) act on the $|v, 2v-3\rangle$ state, Eq. (VI.3.4.) on the $|v, 2v-4\rangle$ state, and Eq. (VI.3.1) on the $|v, 2v-5\rangle$ state, we obtain a set of three linear homogeneous equations in a_1, b_1, c_1 and a similar set of equations in a_2, b_2, c_2, whereby some of the coefficients contain the, at present, unknown eigenvalues $\alpha_{v,2v-6}(i)$ defined by

$$O^0_{2v-6}|v, 2v-6, (i)\rangle = \alpha_{v,2v-6}(i)|v, 2v-6, (i)\rangle. \tag{3.29}$$

We need only to withhold two of these equations in a_1, b_1, c_1 and two in a_2, b_2, c_2, since (3.24) provides us twice with a third relation not containing the unknown eigenvalues. Consequently, the condition which expresses that a_i, b_i, and c_i $(i=1, 2)$ are not all trivially zero, a fact which would be in contradiction with (3.25)–(3.27), is a quadratic equation which has to be satisfied by both $\alpha_{v,2v-6}(1)$ and $\alpha_{v,2v-6}(2)$. This quadratic equation reads

$$\begin{aligned}&x^2-\tfrac{2}{5}\sqrt{2}(16v^4-116v^3+86v^2+194v-165)x \\ &\quad +\frac{2^3}{5^2}(v-2)(v-3)(64v^6-608v^5+228v^4+7352v^3 \\ &\quad -18031v^2+16845v-9450)=0,\end{aligned}$$

and after solving it we can set

$$\begin{aligned}&\alpha_{v,2v-6}(1 \text{ or } 2) \\ &\quad =\tfrac{1}{5}\sqrt{2}[16v^4-116v^3+86v^2+194v-165 \\ &\quad \pm 5(64v^6-960v^5+6832v^4-21312v^3\end{aligned}$$

$$+ 32668v^2 - 26292v + 10161)^{1/2}]. \quad (3.30)$$

The reader can easily verify that for $v = 6$ and $v = 7$ the eigenvalues computed with formula (3.30), correspond to those listed in Table II.2. Solving the system of the mentioned homogeneous equations in a_i, b_i, and c_i, together with the nonhomogeneous equations (3.2.5)–(3.2.7), it can be shown that only for $v = 4$ and $v = 5$, the coefficients a_2, b_2, and c_2 become all zero, a fact which proves that for these seniorities $|v, 2v-6\rangle$ is nondegenerated. Again this is in agreement with the l multiplicities calculated by the aid of group characters, and as such it offers us a nice illustration of the self-consistency of the present technique.

To end this section we give briefly the results associated to the $|v, 2v-7\rangle$ state which is found to be nondegenerated for all $v > 6$ and nonexisting for $v \leqslant 6$

$$\langle v, 2v-4 | O^{+3}_{2v-7} O^{-3}_{2v-4} | v, 2v-4 \rangle = 2^9(v-2)^3(v-3)^2(v-4)(v-5)(v-6) \times (2v-5)^2(4v-3)(4v-5)(4v-7),$$

$$\langle v, 2v-5 | O^{+2}_{2v-7} O^{-2}_{2v-5} | v, 2v-5 \rangle = \frac{2^8}{3}(v-2)(v-3)^2(v-5)(v-6)(2v+1) \times (2v-1)^2(2v-5)^2(4v-7),$$

$$\sum_{i=1}^{2} \langle (i), v, 2v-6 | O^{+1}_{2v-7} O^{-1}_{2v-6} | v, 2v-6, (i) \rangle = \langle v, 2v-7 | O^{-1}_{2v-6} O^{+1}_{2v-7} | v, 2v-7 \rangle = \frac{2^5}{3}(v-3)^2(v-6)(2v-3)(192v^4 - 192v^3 - 492v^2 - 816v + 2055),$$

$$\alpha_{v,2v-7} = \tfrac{2}{5}\sqrt{2}(8v^4 - 74v^3 + 7v^2 + 209v + 15), \quad (v > 6). \quad (3.31)$$

4. DISCUSSION

From the foregoing examples which involve all the aspects of the application of nonscalar product operator relations, it becomes clear that the procedure thereby outlined can be used to generate systematically all O^0_l eigenstates and eigenvalues. Certainly, it cannot be denied that if v is not given a numerical value, but is treated as an arbitrary parameter, the calculations soon become very tedious. However, it is obvious that such calculations can be considerably simplified if it is no longer required to find the l multiplicities by the algorithm itself. Indeed, if there is in advance precise knowledge of the number of existing independent orthonormalized states to be constructed, in most cases the degree of the polynomial equation of which the demanded eigenvalues are solutions, is reduced. Moreover intermediate but at the end meaningless solutions are completely avoided.

It has to be noted that only a restricted class of relations among the set (VI.3.1)–(VI.3.8) has been used in the previous sections, in particular those which ending at $a|v, l\rangle$ state act on states with higher angular momentum than l and do not produce intermediary states with lower angular momentum than l. Certainly, the remaining relations could be invoked as well, but then the eigenvalue calculation of $a|v, l\rangle$ state would have involved eigenvalue calculations of states with lower angular momentum at the same time. Hence, some particular problems associated to tree generation, which we succeeded to avoid by the present technique, would have been reintroduced.

Finally, we like to draw attention to the fact that only shift operator actions lowering the angular momentum, have been witheld for state generation. The reason is that the self-consistent procedure necessarily had to start at the highest angular momentum state, since this is the only state of which the nondegeneracy had not to be proven. Of course, in the point of view that l multiplicities are known in advance, states can be systematically generated from below too. Then we have to take into account the relations which are derived from (VI.3.1)–(VI.3.8) by changing formally l by $-l-1$, and by using the property that $O^{-k}_{-l-1} = O^{+k}_{l}$. As an example, we have calculated the eigenvalues of the doubly degenerated $|v, 6\rangle$ states, where $v = 3k$ and $k > 1$, and we found the following results

$$\langle v, 3 | O^{-3}_{6} O^{+3}_{3} | v, 3 \rangle = 2^{12}3^6 5^2[20v(v+3) - 217],$$

$$\langle v, 4 | O^{-2}_{6} O^{+2}_{4} | v, 4 \rangle = 2^8 3^3 5^3[44v(v+3) - 155],$$

$$\langle v, 3 | O^{-1}_{4} O^{+1}_{3} | v, 3 \rangle = 2^7 \cdot 3 \cdot 5 \cdot 7(2v+1)(2v+5),$$

$$\alpha_{v,6}(1 \text{ or } 2) = 3\sqrt{2}[-15 \pm (1540v(v+3) + 5769)^{1/2}], \quad (v = 3k, \ k > 1). \quad (4.1)$$

The reader can readily verify that $k = 2$ immediately reproduces the numerical values for $\alpha_{6,6}$ listed in Table II.2.

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On a connection between radial Schrödinger equations for different power-law potentials

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A general correspondence is given between the radial Schrödinger equations (in arbitrary dimensions) for confining- and inverse-power law potentials. The wave functions and Green's functions of the two types of potentials are shown to differ by little more than a change of variable (a special case being the well-known equivalence of the harmonic oscillator and Coulomb problems). This gives rise to relationships between the discrete state eigenvalues and matrix elements. Following the lines of a recent paper by Gazeau, the relevance of this correspondence to Sturmian representations for power law potentials is examined. Generalizations are considered for potentials containing a linear combination of powers of r.

I. INTRODUCTION

The technique of changing the independent coordinate has always been a useful tool in the solution of the Scrödinger equation. For one thing, this allows something of a systematic approach, enabling one to recognize the equivalence of superficially unrelated quantum mechanical problems.[1-3] An area where this can be interesting is one-body motion in a central potential. Many recent papers[4-12] have addressed this old subject, and particular emphasis has been placed on the power-law potential[4-10] r^α ($\alpha > -2$), which we will consider in this paper.

Two very special exactly solvable cases of this potential are $\alpha = 2$, the isotropic harmonic oscillator, and $\alpha = -1$, the Coulomb problem. To varying degrees of generality, it has long been recognized that the radial wavefunctions of these two systems can be transformed into each other by a change of coordinates.[13-17] (This applies to the radial Green's functions as well.[18]

Turning our attention to values of the exponent α where we cannot find exact solutions, however, this equivalence is found to be more general in the following sense: The radial Schrödinger equation and its solutions for a potential r^α can be mapped by a change of variable [$r = (c\rho)^\mu$, $\mu = 2/(\alpha+2)$] into those for a potential ρ^β, where $\beta = -2\alpha/(\alpha+2)$. If α is positive, then $-2 < \beta < 0$, and both the α-system and the β-system can possess bound states. The boundary conditions on the two sets of wavefunctions are connected by this transformation, which also preserves the radial node number, giving a one-to-one correspondence of the discrete states. (The angular momenta and dimensionalities, l_α, l_β, D_α, and D_β, are interrelated, but are to some extent arbitrary.) By scaling arguments, simple relations arise between the corresponding energy eigenvalues and diagonal matrix elements.

While the first form of this manuscript was being prepared, papers by Quigg and Rosner[4] and by Gazeau[5] dealing with the same topic were published almost simultaneously. Subsequently, we learned that this equivalence had been studied earlier by Del Guidice and Galzenati,[19] who concentrated on scattering from singular potentials[20] ($\alpha, \beta \leqslant -2$). We try to avoid unnecessary duplication in the following, and would like to point to each of these articles for further information on the subject.

Gazeau[5] has called attention to the fact that the origin of the so-called Sturmian representation[21] is very naturally described by the equivalence mentioned above. Inspired by this, we have examined closely how the Sturmian representation arises for power-law potentials within the context of our more pedestrian approach, and have found that there is a simple generalization to potentials with more than one power of r.

The basic transformation is sketched in Sec. II, leaving arbitrary the dimensionalities of the spaces in which r and ρ are the radial coordinates. By incorporating an explicit rescaling of the new independent variable ρ, we add a degree of freedom to the treatments of Refs. 4 and 5 which will be exploited later. In Secs. III and IV we specialize to the discrete states of attractive potentials, giving the connections between the eigenvalues, matrix elements, and normalizations of the α- and β-systems. In Sec. V the radial Green's functions are also shown to be equivalent. Sec. VI discusses the connection of the earlier results to the wavefunctions and eigenvalues of the Sturmian representation. In Sec. VII, these equivalences and the concept of the Sturmian representation are examined within the context of multiterm potentials.

II. THE BASIC TRANSFORMATION

Our starting point is the radial Schrödinger equation in D dimensions[14]

$$0 = \left[-\frac{\hbar^2}{2m} r^{1-D} \frac{d}{dr} r^{D-1} \frac{d}{dr} + \frac{\hbar^2}{2m} \frac{l(l+D-2)}{r^2} + V(r) - E \right] \psi(r) . \tag{1}$$

Under the substitutions

$$U(r) = \frac{2m}{\hbar^2} V(r) , \tag{2}$$

$$\mathscr{E} = \frac{2m}{\hbar^2} E , \tag{3}$$

$$L = l + \frac{D-2}{2} , \tag{4}$$

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$$\psi(r) = r^{(1-D)/2}\chi(r), \tag{5}$$

we have

$$\left[\frac{d^2}{dr^2} - \frac{L^2 - \frac{1}{4}}{r^2} - U(r) + \mathscr{E}\right]\chi(r) = 0. \tag{6}$$

Equation (5) states that, since $\psi(r)$ has a radial weight function r^{D-1}, $\chi(r)$ has weight function unity. Equation (6) then depends upon l and D only through the parameter L. There is no need to consider l and D separately and, consequently, the number of dimensions is somewhat arbitrary. Actually, we shall regard L as being a continuous parameter from here on,[22] so it is not restricted to the customary integral or half-integral values implied by Eq. (4).

We now specialize to the case of a single-term potential (with a and α constant)

$$U_\alpha(r) = ar^\alpha, \tag{7}$$

and append the subscript α to everything in sight:

$$\left[\frac{d^2}{dr^2} - \frac{L_\alpha^2 - \frac{1}{4}}{r^2} - U_\alpha(r) + \mathscr{E}_\alpha\right]\chi_\alpha(r) = 0. \tag{8}$$

χ_α and the differential equation it satisfies will be called the α-system from now on.

By changing the independent variable from r to ρ,

$$r = (c\rho)^\mu, \tag{9}$$

where c is a rescaling constant, Eq. (8) is transformed into

$$\left\{\frac{d^2}{d\rho^2} + \frac{1-\mu}{\rho}\frac{d}{d\rho} - \mu^2\frac{L_\alpha^2 - \frac{1}{4}}{\rho^2} + \mu^2 c^{2\mu}\rho^{2\mu-2}\left[\mathscr{E}_\alpha - a(c\rho)^{\alpha\mu}\right]\right\}\chi_\alpha((c\rho)^\mu) = 0. \tag{10}$$

This can be written in a form with no first derivatives[23]

$$\left\{\frac{d^2}{d\rho^2} - \frac{\mu^2 L_\alpha^2 - \frac{1}{4}}{\rho^2} + \mu^2 c^{2\mu}\rho^{2\mu-2}\left[\mathscr{E}_\alpha - a(c\rho)^{\alpha\mu}\right]\right\} \times \rho^{(1-\mu)/2}\chi_\alpha((c\rho)^\mu) = 0. \tag{11}$$

This is then *identical* to the equation of the β-system

$$\left[\frac{d^2}{d\rho^2} - \frac{L_\beta^2 - \frac{1}{4}}{\rho^2} - b\rho^\beta + \mathscr{E}_\beta\right]\chi_\beta(\rho) = 0, \tag{12}$$

provided we make the following identifications:

$$\beta = -\frac{2\alpha}{\alpha+2} \quad \left(\alpha = -\frac{2\beta}{\beta+2}\right), \tag{13}$$

$$\mu = \frac{2}{\alpha+2} = \frac{\beta+2}{2}, \tag{14}$$

$$L_\beta = \mu L_\alpha, \tag{15}$$

$$b = -\mu^2 c^{2\mu}\mathscr{E}_\alpha, \tag{16}$$

$$\mathscr{E}_\beta = -\mu^2 c^{(\alpha+2)\mu} a = -\mu^2 c^2 a, \tag{17}$$

and

$$\chi_\beta(\rho) = N\rho^{(1-\mu)/2}\chi_\alpha((c\rho)^\mu). \tag{18}$$

N is just a renormaliation constant, intended to ensure that $\chi_\alpha(r)$ and $\chi_\beta(\rho)$ are normalized in their respective spaces. It is this general relationship that we mean when we use the word equivalence. No distinction has yet been made between the possible boundary conditions or spectra.

The treatments of Refs. 4 and 5 correspond to the choice $c = 1$. As stated in the Introduction, leaving c arbitrary for now gives us an additional degree of freedom. When we discuss bound state eigenvalues later, we can use this to allow the values of the potential coefficients to be completely independent of each other. Note that c may be complex in general, a possibility we ignore. We take c real and positive, and a, b, $\mathscr{E}_\alpha$, and $\mathscr{E}_\beta$ real.

The above relationships are quite circuital. The ranges of α and β break up into three distinct regions:

α	β
$(-\infty, -2)$	$(-\infty, -2)$
$(-2, 0)$	$(0, +\infty)$
$(0, +\infty)$	$(-2, 0)$.

Our interests are mostly in the bound-state spectra. There are no conventional discrete states in the first region,[20] and the last two are redundant due to the symmetry between α and β. Therefore we will only consider the third, with the convention that $-2 < \beta < 0$ and $0 < \alpha < \infty$. This means that Eq. (9) always maps $r = 0$ into $\rho = 0$ and $r = +\infty$ into $\rho = +\infty$.

If attention is further restricted to attractive $U_\beta(\rho)$ ($b < 0$), the spectrum contains a set of discrete states ($\mathscr{E}_\beta < 0$) and a set of continuous ones ($\mathscr{E}_\beta > 0$). Equations (16) and (17) show that these are connected to the discrete states of attractive $U_\alpha(r)$ (a, $\mathscr{E}_\alpha > 0$) and to the continuous states of repulsive $U_\alpha(r)$ ($a < 0$, $\mathscr{E}_\alpha > 0$), respectively. The correspondence of the discrete states is the subject of the next two sections.

III. EXPLICIT CONNECTION BETWEEN BOUND STATE ENERGIES

For fixed L_α, the attractive potential ar^α will have a sequence of bound states indexed by the radial node number n_α ($n_\alpha = 0,1,2,\cdots$), and similarly for attractive $b\rho^\beta$. The corresponding eigenvalues will depend upon the various parameters involved in the differential equations of Sec. II:

$$\mathscr{E}_\alpha = \mathscr{E}_\alpha(a, n_\alpha, L_\alpha), \tag{19}$$

$$\mathscr{E}_\beta = \mathscr{E}_\beta(b, n_\beta, L_\beta). \tag{20}$$

The dependence on α or β is already implied in the subscripts. By the simple nature of the transformation between the wavefunctions, we know that $\chi_\alpha(r)$ and $\chi_\beta(\rho)$ will have the same number of nodes on their respective positive real coordinate axes, so we add to the equations of transformation

$$n_\alpha = n_\beta. \tag{21}$$

From here on we will neglect the subscripts α and β, and uniformly refer to n as the node number.

Equations (16) and (17) must hold for arbitrary choices of a and b, so c is fixed when they are given definite values. Moreover, by eliminating the rescaling constant c between the two equations (remembering that a, $\mathscr{E}_\alpha > 0$ and $b, \mathscr{E}_\beta < 0$), we get

$$-\frac{b}{\mu^2\mathscr{E}_\alpha} = \left[-\frac{\mathscr{E}_\beta}{a\mu^2}\right]^\mu, \tag{22}$$

or, in more symmetrical form,

$$\left[\frac{4\mathscr{E}_\alpha(a,n,L_\alpha)}{(\alpha+2)^2 a^{2/(\alpha+2)}}\right]^\alpha = \left[\frac{4|\,\mathscr{E}_\beta(b,n,L_\beta)|}{(\beta+2)^2|b|^{2/(\beta+2)}}\right]^\beta. \quad (23)$$

The arbitrariness of a and b implies that

$$\mathscr{E}_\alpha = a^{2/(\alpha+2)}\,\mathscr{F}_\alpha(n,L_\alpha), \quad (24)$$

$$\mathscr{E}_\beta = -|b|^{2/(\beta+2)}\,\mathscr{F}_\beta(n,L_\beta), \quad (25)$$

where $\mathscr{F}_\alpha$ and $\mathscr{F}_\beta$ are dimensionless positive functions of the quantum numbers and exponents, and obey

$$\left[\frac{4\mathscr{F}_\alpha(n,L_\alpha)}{(\alpha+2)^2}\right]^\alpha = \left[\frac{4\mathscr{F}_\beta(n,L_\beta)}{(\beta+2)^2}\right]^\beta. \quad (26)$$

Some general hints are given to the dependence of $\mathscr{F}_\alpha$ and $\mathscr{F}_\beta$ on the exponents and quantum numbers in the recent work[4,6,7,9] on level-ordering and WKB treatments for power-law potentials, but only with the Coulomb/harmonic oscillator pair do we have explicit answers (see Appendixes A and B). For general values of α, Eqs. (4) and (15) show that L_α and L_β cannot both be integral or half-integral, the usual case in applications. If we do not require this condition,[22] Eq. (26) may be useful in some calculations by eliminating the need to consider the positive- and negative-exponent regimes separately.

IV. MATRIX ELEMENTS AND NORMALIZATION

In analogy with Louck's treatment[14] of the three-dimensional hydrogen atom and the two-dimensional oscillator, we can relate matrix elements in the α-system to those in the β-system. (The α- and β-dimensionalities need not be specified here, as indicated in the second paragraph in Sec. II.) By Eqs. (16) and (17), for a and b fixed, it is apparent that the rescaling constant c will be different for states of different $\mathscr{E}_\alpha$ (equivalently, states of different $\mathscr{E}_\beta$). The only time that both wavefunctions in an off-diagonal matrix element will rescale by the same constant c will be when an "accidental" degeneracy occurs.[24] Allowing for this case we consider two degenerate states, 1 and 2, and define

$$\langle 1|r^\gamma|2\rangle_\alpha = \int_0^\infty dr\,\chi^*_{\alpha,1}(r)\,r^\gamma\,\chi_{\alpha,2}(r), \quad (27)$$

$$\langle 1|\rho^\nu|2\rangle_\beta = \int_0^\infty d\rho\,\chi^*_{\beta,1}(\rho)\,\rho^\nu\,\chi_{\beta,2}(\rho). \quad (28)$$

The dependence on the quantum numbers and coefficients is being suppressed.

Now from Eqs. (9), (14), and (18),

$$\begin{aligned}\langle 1|r^\gamma|2\rangle_\alpha &= \int_0^\infty d\,((c\rho)^\mu)\,\chi^*_{\alpha,1}((c\rho)^\mu)\,(c\rho)^{\gamma\mu}\,\chi_{\alpha,2}((c\rho)^\mu)\\ &= \frac{1}{N_1^* N_2}\int_0^\infty d\,((c\rho)^\mu)\,\rho^{\mu-1}\,\chi^*_{\beta,1}(\rho)(c\rho)^{\gamma\mu}\,\chi_{\beta,2}(\rho)\\ &= \frac{\mu c^{\mu(\gamma+1)}}{N_1^* N_2}\langle 1|\rho^{\mu(\gamma+2)-2}|2\rangle_\beta\\ &= \frac{\mu c^{\mu(\gamma+1)}}{N_1^* N_2}\langle 1|\rho^{\gamma\mu+\beta}|2\rangle_\beta. \end{aligned} \quad (29)$$

We turn now to the normalization requirement,[25] where states 1 and 2 are the same. If $\chi_{\alpha,1}(r)$ is normalized in r-space, then Eq. (29) for $\gamma = 0$ is

$$1 = \frac{\mu c^\mu}{|N_1|^2}\langle 1|\rho^\beta|1\rangle_\beta. \quad (30)$$

From the virial theorem,

$$\mathscr{E}_{\beta,1} = \mu b\,\langle 1|\rho^\beta|1\rangle_\beta, \quad (31)$$

so

$$|N_1|^2 = \frac{\mathscr{E}_{\beta,1}c^\mu}{b}. \quad (32)$$

Conversely, if $\chi_{\beta,1}(\rho)$ is normalized in ρ-space, then Eq. (29) for $\gamma = -\beta/\mu = \alpha$ is

$$\langle 1|\,r^\alpha|1\rangle_\alpha = \frac{\mu c^{2-\mu}}{|N_1|^2}, \quad (30')$$

or, using the virial theorem again,

$$|N_1|^2 = \frac{ac^{2-\mu}}{\mathscr{E}_{\alpha,1}}. \quad (32')$$

These two forms of $|N_1|^2$ are equivalent by virtue of Eqs. (16) and (17). Note that a weight function of unity in either system corresponds to a weight function of the potential in the other system. (See Ref. 5 and Sec. VI.)

Matrix elements of differential operators may be transformed simply also. One final note: It is possible to write a three-term recursion relation[26–28] for the matrix elements $\langle 1|r^s|2\rangle_\alpha$ with $s = \gamma, \gamma+\alpha$, and $\gamma-2$, and similarly for the β-system (γ is an unspecified constant except that all of the integrals must be finite). If we use Eqs. (29) and (32) and go through the details, the two sets of recursion relations can be shown to be identical, as might have been expected.

V. TRANSFORMATION OF THE GREEN'S FUNCTION

Another remarkable feature of the transformation in Sec. II is that the radial Green's functions, $g_{\alpha,L_\alpha}(r,r';\mathscr{E}_\alpha)$ and $g_{\beta,L_\beta}(\rho,\rho';\mathscr{E}_\beta)$, which satisfy the *inhomogeneous* equations

$$\left\{\frac{d^2}{dr^2} - \frac{L_\alpha^2-\frac{1}{4}}{r^2} - ar^\alpha + \mathscr{E}_\alpha\right\} g_{a,L_\alpha} = \frac{2m_\alpha}{\hbar^2}\delta(r-r'), \quad (33)$$

$$\left\{\frac{d^2}{d\rho} - \frac{L_\beta^2-\frac{1}{4}}{\rho^2} - b\rho^\beta + \mathscr{E}_\beta\right\} g_{\beta,L_\beta} = \frac{2m_\beta}{\hbar^2}\delta(\rho-\rho'), \quad (34)$$

are connected in much the same manner as are χ_α and χ_β.[18]

By making the substitutions

$$r = (c\rho')^\mu, \quad r' = (c\rho')^\mu, \quad (35)$$

and doing a little rearranging in Eq. (33), we have the equation

$$\begin{aligned}&\left\{\frac{d^2}{d\rho^2} - \frac{\mu^2 L_\alpha^2-\frac{1}{4}}{\rho^2} - \mu^2 c^{2\mu}\rho^{2\mu-2}\left[a(c\rho)^{\mu\alpha} - \mathscr{E}_\alpha\right]\right\}\\ &\quad\times(\rho\rho')^{(1-\mu)/2}\,g_{\alpha,L_\alpha}((c\rho)^\mu,(c\rho')^\mu;\mathscr{E}_\alpha)\\ &= \frac{2m_\alpha}{\hbar^2}\mu^2 c^{2\mu}\rho^{2\mu-2}(\rho\rho')^{(1-\mu)/2}\,\delta(c^\mu(\rho^\mu-\rho'^\mu))\\ &= \frac{2m_\alpha}{\hbar^2}\mu c^\mu\,\delta(\rho-\rho'). \end{aligned} \quad (36)$$

In the last step we have used some elementary properties of δ-functions.

Thus, if we insist that Eqs. (13)–(17) hold, we end up with the equivalence

$$g_{\beta,L_\beta}(\rho,\rho';\mathscr{E}_\beta) = M(\rho\rho')^{(1-\mu)/2} g_{\alpha,L_\alpha}\left((c\rho)^\mu,(c\rho')^\mu;\ -\frac{b}{\mu^2}\left[\frac{-\mathscr{E}_\beta}{a\mu^2}\right]^{-\mu}\right). \tag{37}$$

In general $\mathscr{E}_\alpha$ and $\mathscr{E}_\beta$ will be complex, as will c since a and b are real. (g_{α,L_α} and g_{β,L_β} are defined only for the $\mathscr{E}$'s in the complements of the spectra of the original Hamiltonians.) The renormalizing constant M is now determined by requiring that the coefficient of $\delta(\rho-\rho')$ in Eq. (34) be consistent with the result obtained when Eq. (37) is used to write Eq. (36) in terms of g_{β,L_β}, i.e.,

$$M = \frac{m_\beta}{\mu c^\mu m_\alpha}. \tag{38}$$

Other inhomogeneous equations of the α- and β-systems (in one or two variables) can be connected by straightforward generalizations of this section. The equivalence of the Green's functions is particularly interesting, however. The spectral expansion[29] of g_{α,L_α} involves a sum over the complete set of discrete α-wave functions, while g_{β,L_β} is defined in terms of the complete set of β-states, including both discrete *and* continuum wavefunctions.

VI. THE STURMIAN REPRESENTATION FOR POWER-LAW POTENTIALS

There is a close link between the α-β equivalence and the Sturmian technique[21] applied to either system, as Gazeau has emphasized.[5] We want to examine this connection (i) to see how it ties in with our earlier results, and (ii) to pave the way for generalization to more complex potentials in the next section.

We start with a more precise version of Eq. (8)

$$\left[\frac{d^2}{dr^2} - \frac{L_\alpha^2-\frac{1}{4}}{r^2} - ar^\alpha + \mathscr{E}_{\alpha,n}\right]\chi_{\alpha,n}(r) = 0, \tag{39}$$

which emphasizes that, for $a>0$ and $\alpha>0$, there is a complete set of discrete α-states indexed by the radial node number $n=0,1,\cdots$. Since L_α will not change in the following, the dependence of $\mathscr{E}_{\alpha,n}$ and $\chi_{\alpha,n}$ on L_α is suppressed.

If we continued along the lines of Sec. II, the corresponding version of Eq. (9) would now be

$$r = (c_n\rho)^\mu, \tag{40}$$

where c_n is a state-dependent constant, adjusted to convert Eq. (39) to the β-equation

$$\left[\frac{d^2}{d\rho^2} - \frac{L_\beta^2-\frac{1}{4}}{\rho^2} - b\rho^\beta + \mathscr{E}_{\beta,n}\right]\chi_{\beta,n}(\rho) = 0. \tag{41}$$

In this section, we shall call Eqs. (39) and (41) *physical* merely because they are conventional Schrödinger equations, the potential coefficients remaining constant and the energies changing with n.

The path we shall follow here, more along the lines of Refs. 4 and 5, is to demand that $c_n \equiv c$ be independent of n, i.e.,

$$r = (c\rho)^\mu \quad (\text{all } n). \tag{42}$$

Noting that the potentials and energies "switch places" in the transition to the β-system, this will yield an equation in ρ where the potential coefficient varies with n, but the energy does not,

$$\left[\frac{d^2}{d\rho^2} - \frac{L_\beta^2-\frac{1}{4}}{\rho^2} - \lambda_n\, b\rho^\beta + W\right]S_{\beta,n}(\rho). \tag{43}$$

The relevant equations of transformation are Eqs. (13)–(15), (21), (42) and (K_n a constant)

$$\lambda_n b = -\mu^2 c^{2\mu}\mathscr{E}_{\alpha,n}, \tag{44}$$

$$W = -\mu^2 c^2 a, \tag{45}$$

$$S_{\beta,n}(\rho) = K_n\,\rho^{(1-\mu)/2}\chi_{\alpha,n}((c\rho)^\mu). \tag{46}$$

Equation (43) is called *Sturmian*[21] (as opposed to physical) because λ_n instead of W is dependent on n. The $S_{\beta,n}(\rho)$ are wavefunctions of the Sturmian representation for the β-system. Most discussions[21] of these *start* from Eq. (43). Then the "discrete spectrum" is stated to be the set $\{\lambda_n(b,\beta,W,L_\beta)\}$, $n=0,1,2,\cdots$, such that $S_{\beta,n}(\rho)$ has n nodes besides one at the origin and decays exponentially as ρ tends to infinity. By manipulating Eq. (43), it can be shown that

$$(\lambda_n-\lambda_m)\int_0^\infty d\rho\, S^*_{\beta,n}(\rho)\rho^\beta S_{\beta,m}(\rho) = 0, \tag{47}$$

so the $S_{\beta,n}$ can be taken as orthonormal with respect to the weight function ρ^β (or some multiple):

$$\int_0^\infty d\rho\, S^*_{\beta,n}(\rho)\rho^\beta S_{\beta,m}(\rho) = \delta_{n,m}. \tag{48}$$

However, we can just as well arrive at these properties by relating $S_{\beta,n}(\rho)$ to the *physical* $\chi_{\alpha,n}(r)$ [Eq. (46)]. By analogy with Sec. IV, we define

$$\langle n|r^\gamma|m\rangle_{P,\alpha} = \int_0^\infty dr\,\chi^*_{\alpha,n}(r)\,r^\gamma\,\chi_{\alpha,m}(r), \tag{49}$$

$$\langle n|\rho^\nu|m\rangle_{S,\beta} = \int_0^\infty d\rho\, S^*_{\beta,n}(\rho)\rho^\nu S_{\beta,m}(\rho), \tag{50}$$

where the subscripts P and S denote physical and Sturmian, respectively. Since all states transform under the same change of variable here, we obtain an equation much like Eq. (29), but valid for all node numbers n and m,

$$\langle n|r^\gamma|m\rangle_{P,\alpha} = \frac{\mu c^{\mu(\gamma+1)}}{K_n^* K_m}\langle n|\rho^{\gamma\mu+\beta}|m\rangle_{S,\beta}. \tag{51}$$

For $\gamma=0$, we have (assuming orthonormality of the χ_α's)

$$\langle n|m\rangle_{P,\alpha} = \delta_{n,m} = \frac{\mu c^\mu}{K_n^* K_m}\langle n|\rho^\beta|m\rangle_{S,\beta}. \tag{52}$$

Equation (48) requires that

$$|K_n|^2 = \mu c^\mu, \tag{53}$$

so the coefficient on the right-hand side of Eq. (51) can be reduced to $c^{\mu\gamma}$ if all K_n have the same phase.

The interesting point here is that the complete set of physical α-states corresponds exactly to the complete set of Sturmian β-states. Orthonormality of the Sturmian functions with weight function ρ^β [Eqs. (47) and (48)] can be viewed as a consequence of the orthonormality of the phys-

ical α-functions with weight function unity.

Some particularly simple results occur when $W = \mathscr{E}_{\beta,n'}$, the physical eigenvalue of Eq. (41) for some n'. Then Eq. (45) shows that $c = c_{n'}$, the rescaling constant that takes $\chi_{\alpha,n'}(r)$ into $\chi_{\beta,n'}(\rho)$. The $\chi_{\beta,n}(\rho)$ and $S_{\beta,n}(\rho)$ differ in their scaling except for the single case, $n = n'$.[21]

Note that the Sturmian eigenvalue simplifies also. Eliminating c between Eqs. (44) and (45), setting $W = \mathscr{E}_{\beta,n'}$ and using Eq. (22),

$$\lambda_n b = -\mu^2 \mathscr{E}_{\alpha,n} \left[\frac{-W}{\mu^2 a}\right]^{\mu}\Bigg|_{W=\mathscr{E}_{\beta,n'}} = \frac{\mathscr{E}_{\alpha,n}}{\mathscr{E}_{\alpha,n'}} b\,. \tag{54}$$

Thus the Sturmian eigenvalues are related straightforwardly to the physical α-eigenvalues, and reduce to unity for the case $n = n'$.

As a remark about the symmetry between the α- and β-systems, it follows quite analogously that the Sturmian α-states correspond to the physical β-states (both of which also have continuous spectra). For the case of the simple power-law potential, the Sturmian representations can be studied more directly by scaling than by using the α-β equivalence as an intermediary, but the latter approach provides another interpretation of where the Sturmian states come from, and will be helpful in the next section.

VII. MULTITERM POTENTIALS

Suppose we have the equation

$$\left[\frac{d^2}{dr^2} - \frac{L_\alpha^2 - \frac{1}{4}}{r^2} - U_\alpha(r) + \mathscr{E}_\alpha\right]\chi_\alpha(r) = 0\,, \tag{55}$$

where U_α is a general sum of distinct powers of r

$$U_\alpha(r) = \sum_i a_i r^{\alpha_i} \quad (\alpha_i > -2)\,. \tag{56}$$

Pick a particular exponent, say α_k, and change the independent coordinate to ρ:

$$r = (c\rho)^{\mu_k}\,, \tag{57}$$

with

$$\mu_k = \frac{2}{\alpha_k + 2}\,. \tag{58}$$

Then, just as in Sec. II, Eq. (55) can be transformed into

$$\left[\frac{d^2}{d\rho^2} - \frac{L_\beta^2 - \frac{1}{4}}{\rho^2} - U_\beta(\rho) + \mathscr{E}_\beta\right]\chi_\beta(\rho) = 0\,, \tag{59}$$

where

$$U_\beta(\rho) = \sum_i b_i \rho^{\beta_i}\,, \tag{60}$$

and the following substitutions have been made:

$$\chi_\beta(\rho) = N\rho^{(1-\mu_k)/2}\chi_\alpha((c\rho)^{\mu_k})\,, \tag{61}$$

$$L_\beta = \mu_k L_\alpha\,, \tag{62}$$

$$\mathscr{E}_\beta = -\mu_k^2 c^2 a_k\,, \tag{63}$$

$$b_k = -\mu_k^2 c^{2\mu_k}\mathscr{E}_\alpha\,, \tag{64}$$

$$b_i = \mu_k^2 c^{\mu_k(\alpha_i+2)} a_i \quad (i \neq k)\,, \tag{65}$$

$$\beta_k = 2\mu_k - 2 = -\frac{2\alpha_k}{\alpha_k + 2}\,, \tag{66}$$

$$\beta_i = \mu_k(\alpha_i + 2) - 2 = \frac{2(\alpha_i - \alpha_k)}{\alpha_k + 2} \quad (i \neq k)\,. \tag{67}$$

The $a_k r^{\alpha_k}$ term has become $\mathscr{E}_\beta$, while the $\mathscr{E}_\alpha$ term has taken up the position k in $U_\beta(\rho)$. These transformations are again circuital, since

$$\alpha_k = -\frac{2\beta_k}{\beta_k + 2}\,, \tag{68}$$

$$\alpha_i = \frac{2(\beta_i - \beta_k)}{\beta_k + 2} \quad (i \neq k)\,. \tag{69}$$

Also, if all $\alpha_i > -2$, it follows that all $\beta_i > -2$.

It is apparent from the above that, as the number of terms in $U_\alpha(r)$ grows, so does the number of related systems (different choices of α_k). Matters now depend in an involved way on the signs *and* relative magnitudes of the potential coefficients, both of which will determine whether or not discrete states may exist. A given potential $U_\alpha(r)$ may be attractive in some regions and repulsive in others. (Resonances may appear, but these will be associated with complex energies and fall outside the scope of this paper.)

Moreover, even if there are discrete states for a given $U_\alpha(r)$ (that is, all of the α_i's are fixed), we see from Eqs. (63)–(65) an important distinction from the single-term case. Different values of $\mathscr{E}_\alpha$ will always yield different values of the b_i's, so that $U_\beta(\rho)$ will depend on *which* eigenvalue $\mathscr{E}_\alpha$ is chosen. A physical α-system cannot correspond to a physical β-system, in the sense of Sec. VI, for more than one state.[30] State-by-state, of course, the previous sections can be generalized to the multiterm potentials if desired.

What does carry over from the single-term potential, however, is the correspondence of Sturmian and physical representations. If the same value of c is used for all $\mathscr{E}_\alpha$ in the transformations of this section, Eqs. (63)–(65) show that $\mathscr{E}_\beta$ and every b_i except b_k remain constant, b_k varying linearly with $\mathscr{E}_\alpha$. Thus the physical α-system gives rise to a Sturmian β-system with weight function ρ^{β_k}, and matrix elements can again be equated between the two systems. The discrete Sturmian eigenvalues are now the values of the coefficient b_k which, for fixed $\mathscr{E}_\beta$ and $b_i (i \neq k)$, give rise to bound states.

The β-system can conversely be taken as the physical one instead of the α-system. This will lead to quantization of a_k for fixed $\mathscr{E}_\alpha$ and $a_i (i \neq k)$. For each term in $U_\alpha(r)$, there is an *individual* Sturmian representation which can be put into correspondence with a physical β-representation, generated by choosing the appropriate exponent α_k in the preceding. Put briefly, quantization of any coupling constant a_k in $U_\alpha(r)$ is exactly the same as quantization of the energy in another system.

As an example of "equivalent" sets of exponents, consider a potential $U_\alpha(r)$ with three terms, $\alpha_1 = -1$, $\alpha_2 = +1$, and $\alpha_3 = +2$. For $L_\alpha = \frac{1}{2}$ and for special choices of the coefficients, this problem has an exact eigensolution.[31]

Taking $k = 1$, 2, and 3 gives us the following values of the β_i's:

	$k=1$	$k=2$	$k=3$
β_1	2	$-\frac{4}{3}$	$-\frac{3}{2}$
β_2	4	$-\frac{2}{3}$	$-\frac{1}{2}$
β_3	6	$+\frac{2}{3}$	-1

The $k = 1$ choice, which is the one involved in the Coulomb-to-oscillator transformation, shows that the β-system is that of a generalized anharmonic oscillator.[32]

If we drop the α_3 term, we have the Coulomb-plus-linear term potential of recent interest,[4] and we ignore the third row and column above. The $k = 1$ choice now corresponds to a radial oscillator-with-quartic-term potential. Outside the context of radial problems, this anharmonic oscillator has also been noted as equivalent to the system of equations involved in the parabolic coordinate treatment[33,34] of the hydrogen atom Stark effect.

Another example is provided by Stillinger,[11] who shows how the two-term potentials $(\alpha_1,\alpha_2) = (-1, -\frac{1}{2}), (-\frac{2}{3},\frac{2}{3})$ and (1,2) can all be solved in terms of parabolic cylinder functions for special choices of the coefficient of r^{-2}. These fall within the purview of the above transformations, any two pairs being generated by the third.

VIII. CONCLUSION

By changing the independent variable in the radial Schrödinger equation, we have been able to demonstrate a close equivalence between positive- and negative-power single term potentials. This equivalence encompasses wavefunctions, matrix elements, eigenvalues and Green's functions. Scaling arguments have formed our major point of departure from similar recent treatments.

We have superficially investigated potentials with an arbitrary number of powers of r. For such potentials, the variable change has been used to provide an interpretation of Sturmian equations in terms of ordinary physical Schrödinger equations.[5] From the mathematical standpoint of quantization, the coupling constants and the energy are on very much the same footing (see Ref. 12 for an ingenious application; see also Appendix C).

It should be mentioned that recognition of the equivalences among power-law potentials has been useful in expanding the function $\chi_\alpha(r)$ in Eq. (8) [and even the $\chi_\alpha(r)$ in Eq. (55)] about the origin.[35] This is of no help in eigenvalue determination, of course, unless some means of incorporating the boundary condition of exponential decay at infinity can be found.[36] Whether or not the equivalences have anything to say about asymptotic expansions of the wavefunctions is an open question, although it appears doubtful.

The relationship between the α- and β-systems is presumably reflected in perturbation theory. Considering just the Coulomb/harmonic oscillator pair, for which we are more or less in a position to do the calculations, Sec. VII shows that we can add terms to each Hamiltonian so that the new radial equations still correspond for at least one state. It would be interesting to see how the perturbation developments compare.

Another avenue we have not explored is the significance of these transformations for resonance wavefunctions. For instance, one may have a "Sturmian resonance," where one of the potential coefficients is complex, and the energy and all other coefficients are real. It might be profitable to employ the complex coordinate rotation method[37] here, that is, allowing the rescaling constant c to be complex. This is a step beyond our relatively harmless transformation with real c, which had the property of preserving the nodal structure of the wavefunctions.

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APPENDIX A: COULOMB AND HARMONIC OSCILLATOR WAVEFUNCTIONS

In the present notation, the bound-state $\alpha = 2$ and $\beta = -1$ wavefunctions are[14,38]

$$\chi_2(r) = \left[\frac{2\xi n_2!}{\Gamma(n_2 + L_2 + 1)}\right]^{1/2} \times (\xi r)^{L_2 + 1/2} e^{-(\xi r)/2} \mathscr{L}^{L_2}_{n_2}(\xi^2 r^2) \quad (\xi = a^{1/4}), \tag{A1}$$

$$\chi_{-1}(\rho) = \left[\frac{\xi^2 n_{-1}!}{2\Gamma(n_{-1} + 2L_{-1} + 1)}\right]^{1/2} (-b)^{-1/2} (\xi\rho)^{L_{-1}+1/2} \times e^{-\xi\rho/2} \mathscr{L}^{2L_{-1}}_{n_{-1}}(\xi\rho) \quad \left(\xi = -\frac{b}{n_{-1} + L_{-1} + \frac{1}{2}}\right), \tag{A2}$$

with associated eigenvalues

$$\mathscr{E}_2 = 2a^{1/2}[2n_2 + L_2 + 1], \tag{A3}$$

and

$$\mathscr{E}_{-1} = -\frac{(-b)^2}{4}[n_{-1} + L_{-1} + \tfrac{1}{2}]^{-2}. \tag{A4}$$

The functions $\mathscr{L}^{\mu}_{n}(x)$ in Eqs. (A1) and (A2) are associated Laguerre polynomials, defined as[39]

$$\mathscr{L}^{\mu}_{n}(x) = \sum_{i=0}^{n} \frac{(-x)^i}{i!}\binom{n+\mu}{n-i}. \tag{A5}$$

By use of Eqs. (9), (13)–(17), (21), and (22), it is easy to show that these wavefunctions are related by Eq. (18). In establishing a connection with the normal terminology, it must be remembered that we have scaled the potentials and energies [cf. Eqs. (2) and (3)].

In Appendix B we will want the quantities [see Eqs. (24) and (25)]

$$\mathscr{F}_2(n_2,L_2) = 4\left[n_2 + \frac{L_2+1}{2}\right], \tag{A6}$$

and

$$\mathscr{F}_{-1}(n_{-1},L_{-1}) = \tfrac{1}{4}(n_{-1}+L_{-1}+\tfrac{1}{2})^{-2}. \tag{A7}$$

APPENDIX B: DERIVATIVES $\mathscr{E}_\alpha$ AND $\mathscr{E}_\beta$

The Hellman–Feynman theorem[40] tells us that, for instance,

$$\left(\frac{\partial \mathscr{E}_\alpha}{\partial \alpha}\right)_{a,n_\alpha,L_\alpha} = a\langle \chi_\alpha | r^\alpha \ln r | \chi_\alpha \rangle_\alpha . \tag{B1}$$

If we naively assume analyticity in the exponents near $\alpha = 2$ and $\beta = -1$ we can use the wavefunctions in Appendix A to calculate [$a>0$, $\psi(x) = (d/dx)\ln\Gamma(x)$]

$$\left(\frac{\partial \mathscr{E}_\alpha}{\partial \alpha}\right)_{a,n_\alpha,L_\alpha}\Bigg|_{\alpha=2} = a^{1/2}\left\{n_2+\tfrac{1}{2}+\left(n_2+\frac{L_2+1}{2}\right)[\psi(n_2+L_2+1)-\tfrac{1}{2}\ln a]\right\}, \tag{B2}$$

and ($\zeta = -b/(n_{-1}+L_{-1}+\tfrac{1}{2}) > 0$)

$$\left(\frac{\partial \mathscr{E}_\beta}{\partial \beta}\right)_{b,n_\beta,L_\beta}\Bigg|_{\beta=2} = -\frac{\zeta^2}{2}\{\psi(n_{-1}+2L_{-1}+1)-\ln\zeta\}. \tag{B3}$$

We can eliminate the contributions to these derivatives from the coefficients a and b by use of Eqs. (24) and (25). The end result is

$$\left(\frac{\partial \mathscr{F}_\alpha}{\partial \alpha}\right)_{n_\alpha,L_\alpha}\Bigg|_{\alpha=2} = n_2+\tfrac{1}{2}+\left(n_2+\frac{L_2+1}{2}\right)\psi(n_2+L_2+1), \tag{B4}$$

and

$$\left(\frac{\partial \mathscr{F}_\beta}{\partial \beta}\right)_{n_\beta,L_\beta}\Bigg|_{\beta=-1} = \frac{1}{2[n_{-1}+L_{-1}+\tfrac{1}{2}]^2} \times [\psi(n_{-1}+2L_{-1}+1) + \ln(n_{-1}+L_{-1}+\tfrac{1}{2})]. \tag{B5}$$

If not the accuracy, at least the consistency of Eqs. (B4) and (B5) can be checked by use of Eqs. (13), (15), and (26), remembering that L_α and L_β are not simultaneously held fixed. In principle second derivatives can be calculated, but these do not appear to be expressible in closed form.

Note the evidence of some Γ-function structure (or a generalization thereof) in $\mathscr{F}_\alpha$ and $\mathscr{F}_\beta$ which must simplify drastically at the values $\alpha = 2$ and $\beta = -1$ [see Eqs. (A6) and (A7)]. This is in agreement with the WKB development. However, the very nice zeroth-order WKB treatment of Feldman, Fulton, and Devoto[7] implies that ($N_\alpha = n_\alpha + \tfrac{1}{2}$)

$$\mathscr{F}_\alpha(N_\alpha,L_\alpha) = \left[A\left(\frac{N_\alpha}{L_\alpha},\alpha\right)N_\alpha + B\left(\frac{N_\alpha}{L_\alpha},\alpha\right)L_\alpha\right]^{2\alpha/(\alpha+2)}, \tag{B6}$$

where A and B are unspecified functions of their arguments. This form of $\mathscr{F}_\alpha$, and the analogous one for $\mathscr{F}_\beta$, are reasonably good approximations for power-law potentials, and exact for $\alpha = 2$ and $\beta = -1$. Moreover, it can be shown to conform with Eq. (26). Differentiation of Eq. (B6) with respect to α will give a term in $\mathscr{F}_\alpha \ln(\mathscr{F}_\alpha)$, however, and yet there is no term at all involving the logarithm of the quantum numbers in Eq. (B4). The author is not sure of the source of this discrepancy, although it is tempting to blame the approximate nature of Eq. (B6).[41]

APPENDIX C: THE SEMICLASSICAL POINT OF VIEW

Feldman, Fulton, and Devoto[7] have shown recently that the leading-order WKB integrals are essentially identical for the α- and β-systems. The higher-order corrections[42,43] are currently being investigated, but we now know that the α- and β-integrals of the WKB method should correspond in each order in $\hbar$ since the exact quantum mechanical treatments do.

A few words are appropriate here for a different perspective on the α-β equivalence. Radial WKB problems on the semi-infinite interval $(0,\infty)$ necessitate use of the Langer transformation[44–46]

$$r = e^x, \tag{C1}$$

$$\chi_\alpha(r) = e^{x/2}\phi_\alpha(x). \tag{C2}$$

Equation (8) becomes

$$\left[\frac{d^2}{dx^2} + \mathscr{E}_\alpha e^{2x} - ae^{(\alpha+2)x} - L_\alpha^2\right]\phi_\alpha(x) = 0. \tag{C3}$$

If the β-system is handled analogously, then

$$\rho = e^y, \tag{C4}$$

$$\chi_\beta(\rho) = e^{y/2}\phi_\beta(y), \tag{C5}$$

$$\left[\frac{d^2}{dy^2} + \mathscr{E}_\beta e^{2y} - be^{(\beta+2)y} - L_\beta^2\right]\phi_\beta(y) = 0. \tag{C6}$$

The transformation $r = (c\rho)^\mu$ becomes

$$x = \mu(y + \ln c), \tag{C7}$$

i.e., merely a change of scale and origin of the independent variable. (Note that this causes the "eigenvalue" L_α^2 to be multiplied by μ^2.) Other than these differences, the WKB treatments will be identical. This also serves to demonstrate the symmetrical roles of the energy and the coupling constant mentioned by Gazeau.[5] In this framework, they both appear as coupling constants.

Another interesting, though possibly already known, feature of the Langer transformation is that it carries the complex coordinate rotation method into the recently introduced coordinate translation approach.[47] This just means that giving r a phase in Eq. (C1) ($r \to r e^{i\theta}$) is equivalent to translating x off the real axis ($x \to x + i\theta$). As far as the α-β transformation goes, this can be accomplished by making c complex, thus introducing an imaginary additive term to Eq. (C7).

Added in Proof. Yet another discussion of the transformation considered in this paper, discovered after submission of the manuscript, may be found in A. Joseph, Int. J. Quant. Chem. **1**, 615 (1967).

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$$G(\mathbf{r}_1,\mathbf{r}_2,k) = \frac{1}{2\pi}\sum_{m=-\infty}^{\infty} e^{im(\phi_1-\phi_2)} G_m(\xi_1,\xi_2,\eta_1\eta_2,k).$$
Interestingly enough, the transformation of Ref. 33 can be used as in Sec. V to show that $G_m(\xi_1,\eta_1,\xi_2,\eta_2,k)$ is equivalent to the radial Green's function of two identical, noninteracting, two-dimensional harmonic oscillators, both with the same value of the angular momentum.
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Formal solutions of inverse scattering problems. III

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The formal solutions of certain three-dimensional inverse scattering problems presented in papers I and II of this series [J. Math. Phys. **10**, 1819 (1969); **17** 1175 (1976)] are obtained here as fixed points of a certain nonlinear mapping acting on a suitable Banach space of integral kernels. When the scattering data are sufficiently restricted, this mapping is shown to be a contraction, thereby establishing the existence, uniqueness, and continuous dependence on the data of these formal solutions.

I. INTRODUCTION

In part I[1] of this series formal solutions of certain three-dimensional scattering problems were developed from a procedure suggested by Jost and Kohn[2] and developed by Moses.[3] In part II[4] these formal solutions were shown, under suitably restricted hypotheses, to converge to true solutions to some of these problems. These solutions were not shown, however, to be unique or consistent with one another.

In this paper these questions are settled by establishing a new procedure which obtains the same solutions as fixed points of a certain nonlinear mapping acting on a suitable Banach space of integral kernels. At the same time the new procedure also obtains the full scattering matrix from the given scattering data. When the data are sufficiently restricted, this mapping is shown to be a contraction, thereby establishing the existence, uniqueness, and continuous dependence on the data of the solutions.

As in parts I and II, three classes of problems are considered separately: problems of potential scattering, refractive scattering, and boundary scattering.

2. POTENTIAL SCATTERING

The scattering of a quantum-mechanical wave function $\varphi(\mathbf{x},\mathbf{k})$ from a fixed potential function $V(\mathbf{x})$ is governed by the time-independent Schrödinger equation,

$$(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = V(\mathbf{x})\varphi(\mathbf{x},\mathbf{k}), \quad \mathbf{x},\mathbf{k}\in\mathbb{R}^3 . \tag{1}$$

The solution, which is to consist of an ingoing plane wave plus an outgoing scattered wave, may be expressed as

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \int \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} V(\mathbf{y})\varphi(\mathbf{y},\mathbf{k})\, d\mathbf{y} . \tag{2}$$

As $|\mathbf{x}|\to\infty$ the behavior of $\varphi(\mathbf{x},\mathbf{k})$ is given by

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{e^{i|\mathbf{k}||\mathbf{x}|}}{4\pi|\mathbf{x}|} T(\mathbf{k}',\mathbf{k}) + O\left(\frac{1}{|\mathbf{x}|^2}\right). \tag{3}$$

Here $\mathbf{k}' = (|\mathbf{k}|/|\mathbf{x}|)\mathbf{x}$, and $T(\mathbf{k}',\mathbf{k})$ is given by

$$T(\mathbf{k}',\mathbf{k}) = \int e^{-i\mathbf{k}'\cdot\mathbf{y}} V(\mathbf{y})\varphi(\mathbf{y},\mathbf{k})\, d\mathbf{y}. \tag{4}$$

Thus $T(\mathbf{k}',\mathbf{k})$ contains the scattering data. Expression (4) makes sense for arbitrary $\mathbf{k}',\mathbf{k}\in\mathbb{R}^3$, and leads to an iterative solution for $T(\mathbf{k}',\mathbf{k})$ obtained by first solving (2) for $\varphi(\mathbf{x},\mathbf{k})$ and then substituting the result in (4):

$$\begin{aligned} T(\mathbf{k}',\mathbf{k}) = &\int e^{-i\mathbf{k}'\cdot\mathbf{y}} V(\mathbf{y}) e^{i\mathbf{k}\cdot\mathbf{y}}\, d\mathbf{y} \\ &- \int\int e^{-i\mathbf{k}'\cdot\mathbf{y}_1} V(\mathbf{y}_1) \frac{e^{i|\mathbf{k}||\mathbf{y}_1-\mathbf{y}_2|}}{4\pi|\mathbf{y}_1-\mathbf{y}_2|} \\ &\times V(\mathbf{y}_2) e^{i\mathbf{k}\cdot\mathbf{y}_2}\, d\mathbf{y}_2\, d\mathbf{y}_1 + \cdots . \end{aligned} \tag{5}$$

If Fourier transforms are taken throughout, then

$$\begin{aligned} T(\mathbf{k}',\mathbf{k}) = &V(\mathbf{k}',\mathbf{k}) \\ &- \int V(\mathbf{k}',\mathbf{k}'')(\mathbf{k}''^2 - \mathbf{k}^2 + i0)^{-1} V(\mathbf{k}'',\mathbf{k})\, d\mathbf{k}'' \\ &+ \cdots , \end{aligned} \tag{6}$$

or, more formally,

$$T = V - V(\Gamma V) + V(\Gamma V(\Gamma V)) + \cdots , \tag{7}$$

where, for any integral kernel K, ΓK is the kernel

$$\Gamma K(\mathbf{k}',\mathbf{k}) = (\mathbf{k}'^2 - \mathbf{k}^2 + i0)^{-1} K(\mathbf{k}',\mathbf{k}) . \tag{8}$$

Now if we can choose an appropriate class of integral kernels containing $V(\mathbf{k}'-\mathbf{k})$ and define a norm of Friedrichs type for this class[5,6] such that $\|K\Gamma M\| \leqslant \|K\|\|M\|$ and such that

$$\|V\| = a < 1 , \tag{9}$$

then the series (7) for T converges to T in this norm, and

$$\|T\| \leqslant a(1-a)^{-1} . \tag{10}$$

Moreover, if V and V' are two potential kernels, both satisfying (9), and T and T' are the corresponding scattering kernels obtained through (7), then the difference $T - T'$ satisfies

$$\begin{aligned} T - T' = &V - V' - ((V-V')\Gamma V + V'\Gamma(V-V')) \\ &+ ((V-V')\Gamma V\Gamma V + V'\Gamma(V-V')\Gamma V \\ &+ V'\Gamma V'\Gamma(V-V')) + \cdots , \end{aligned} \tag{11}$$

so that, if (9) holds, then

$$\begin{aligned} \|T - T'\| &\leqslant (1 + 2a + 3a^2\cdots)\|V - V'\| \\ &= (1-a)^{-2}\|V - V'\| . \end{aligned} \tag{12}$$

Thus the (nonlinear) mapping $\Phi: V\to T$ is defined and continuous on the space of potential kernels satisfying (9).

To invert this mapping, we proceed as follows. From (7) we have

$$T = V - V\Gamma T = VU , \tag{13}$$

where

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$$U = 1 - \Gamma T, \tag{14}$$

is the kernel for the ingoing Möller wave matrix. This operator is known to be unitary for a large class of potentials V provided there are no bound states in the problem.[5] In particular, U is unitary if (9) holds, and we may write

$$UU^* = I, \tag{15}$$

with

$$U^* = 1 + \Gamma T^*, \tag{16}$$

where, as usual $T^*(\mathbf{k}',\mathbf{k}) = \overline{T}(\mathbf{k},\mathbf{k}')$ is the kernal adjoint to $T(\mathbf{k}',\mathbf{k})$. Applying (15) to (13), we find

$$V = VUU^* = TU^* = T + T\Gamma T^*, \tag{17}$$

which gives the potential kernel $V(\mathbf{k}' - \mathbf{k})$ directly in terms of the full scattering kernel $T(\mathbf{k}',\mathbf{k})$.

Everything done so far works just as well if the original potential is nonlocal, in which case the potential kernel has the more general form $V(\mathbf{k}',\mathbf{k})$ instead of the convolution form $V(\mathbf{k}' - \mathbf{k})$. It follows from the discussion above that the (nonlinear) mapping $\Phi: V \to T$ is continuously defined by (7) on the space of *all* potential kernels $V(\mathbf{k}',\mathbf{k})$, local or not, satisfying $\|V\| < 1$, with continuous inverse defined by (13) or (17) on the space of *all* scattering kernels $T(\mathbf{k}',\mathbf{k})$ satisfying $\|T\| < 1$.

In practice, however, the observable scattering data determine only a part of the full scattering kernel $T(\mathbf{k}',\mathbf{k})$. It follows from (3), in particular, that observable data can determine $T(\mathbf{k}',\mathbf{k})$ only for $|\mathbf{k}'| = |\mathbf{k}|$ (the "on-shell" values), while the construction of a potential $V(\mathbf{k}',\mathbf{k})$ via (13) or (17) requires $T(\mathbf{k}',\mathbf{k})$ for *all* values of $(\mathbf{k}',\mathbf{k})$ (including "off-shell" values). We conclude that the inverse problem for *general* potentials has no general solution.

For *local* potentials, however, we might expect that the off-shell values of $T(\mathbf{k}',\mathbf{k})$ are somehow determined by on-shell values. In fact, to reconstruct (the three-parameter set of values of) a local potential, we should need only a three-parameter set of scattering data. From this point of view then, the inverse scattering problem for local potentials is to reconstruct the full scattering kernel $T(\mathbf{k}',\mathbf{k})$ from some suitable three-parameter subset of observable scattering data, and then use (13) or (17). We shall see that at least for weak local potentials, this problem has a nice solution.

Suppose now that $T(\mathbf{k}',\mathbf{k})$ is obtained from a local potential $V(\mathbf{k}' - \mathbf{k})$, and suppose we know all the *backscattering* data, i.e., all the values of $T(\mathbf{k}',\mathbf{k})$ when $\mathbf{k}' = -\mathbf{k}$. We ask whether $T(\mathbf{k}',\mathbf{k})$ can be reconstructed from $T(-\mathbf{k},\mathbf{k})$.

To examine this question, we set $\mathbf{h} = \mathbf{k}' = -\mathbf{k}$, and define the function

$$B(2\mathbf{h}) = T(\mathbf{h}, -\mathbf{h}) = T(-\mathbf{k},\mathbf{k}). \tag{18}$$

Then $B(2\mathbf{h})$ is completely determined by the backscattering data, and determines, in turn, a convolution kernel

$$B(\mathbf{h}' - \mathbf{h}) = T\left(\frac{\mathbf{h}' - \mathbf{h}}{2}, \frac{\mathbf{h} - \mathbf{h}'}{2}\right), \tag{18a}$$

which, as we shall see, determines $T(\mathbf{k}',\mathbf{k})$.

We now define an operation Θ which projects the integral kernels in our Friedrichs class onto the convolution kernels according to the formula

$$\Theta K(\mathbf{k}' - \mathbf{k}) = K\left(\frac{\mathbf{k}' - \mathbf{k}}{2}, \frac{\mathbf{k} - \mathbf{k}'}{2}\right). \tag{19}$$

We verify immediately, as in Ref. 4, that

$$\Theta V(\mathbf{k}' - \mathbf{k}) = V(\mathbf{k}' - \mathbf{k}), \tag{20}$$

$$\Theta T(\mathbf{k}' - \mathbf{k}) = B(\mathbf{k}' - \mathbf{k}), \tag{21}$$

$$\Theta^2 K(\mathbf{k}' - \mathbf{k}) = \Theta K(\mathbf{k}' - \mathbf{k}), \tag{22}$$

$$\|\Theta K\| \leqslant \|K\|, \tag{23}$$

so that Θ is indeed a projection upon the convolution kernels in our Friedrichs class.

We note that the mapping $\Theta\Phi: V \to B$ is defined and continuous from the space of local potential kernels satisfying (9) into the space of backscatter kernels satisfying (10). It is this mapping which we now wish to invert.

Inserting (20) and (21) into (17), we obtain

$$V = \Theta V = \Theta T + \Theta T\Gamma T^* = B + \Theta T\Gamma T^*. \tag{24}$$

Inserting (24) in turn into (17) and solving for T, we finally obtain

$$T = B - (1 - \Theta)T\Gamma T^*. \tag{25}$$

Thus we see that if V is a local potential satisfying (9) then the corresponding scattering kernel T obtained through (7) must satisfy the (nonlinear) integral Eq. (25). Conversely, if the scattering kernel T satisfies (9) and (25), then the corresponding potential obtained through (17) must be local, since if $V = T + T\Gamma T^*$, then $\Theta V = B + \Theta(T\Gamma T^*)$, and from (25), $B + \Theta(T\Gamma T^*) = T + T\Gamma T^* = V$. Hence, Eq. (25) *characterizes the scattering kernels obtained from local potentials satisfying* (9). Moreover, the mapping $\Theta: V \leftrightarrow T$ carries the space of local potentials satisfying (9) one-to-one and bicontinuously *into* the space of backscattering kernels T satisfying (25) and (10), and, by (17), *onto* the subspace of T satisfying (25) with $\|T\| \leqslant a/2$.

We now show that Eq. (25) has a unique solution giving the scattering kernel $T(\mathbf{k}',\mathbf{k})$ in terms of the backscattering kernel $B(\mathbf{k}' - \mathbf{k})$, provided $B(\mathbf{k}' - \mathbf{k})$ is not too big in the Friedrichs norm:

$$\|B\| \leqslant b < \tfrac{1}{8}. \tag{26}$$

Under this assumption we examine the nonlinear mapping of integral kernels $K(\mathbf{k}',\mathbf{k})$ defined by

$$F(K) = B - (1 - \Theta)K\Gamma K^*. \tag{27}$$

We first observe that if

$$\|K\| \leqslant 2b < \tfrac{1}{4}, \tag{28}$$

then

$$\begin{aligned} \|F(K)\| &\leqslant \|B\| + 2\|K\|\|K^*\| \\ &\leqslant b + 8b^2 \\ &\leqslant 2b \text{ if } b < \tfrac{1}{8}. \end{aligned} \tag{29}$$

Moreover, if B and B' are obtained from two sets of backscatter data, and if F and F' are the corresponding mappings, and K and K' are any two kernels satisfying (28), then

$$\begin{aligned} F(K) - F'(K') = B - B' - (1 - \Theta)((K - K')\Gamma K^* \\ + K'\Gamma(K - K')^*), \end{aligned} \tag{30}$$

so that

$$\|F(K)-F'(K')\|\leqslant\|B-B'\|+8b\,\|K-K'\|\,. \tag{31}$$

In particular, if $B=B'$ and if $8b<1$, then (29) and (31) say that F is a contraction mapping on the space of kernels satisfying (28), and the Banach contraction mapping principle applies.[7]

According to this principle, the equation

$$F(K)=K \tag{32}$$

has a unique solution in the space of kernels satisfying (28), and this solution may be obtained iteratively from any zeroth approximation satisfying (28). Thus if

$$\|K_0\|\leqslant 2b\,, \tag{33}$$

$$K_{n+1}=F(K_n)\,, \tag{34}$$

then $K_n\to K$, $F(K)=K$, and

$$\|K-K_n\|\leqslant\tfrac{1}{2}(8b)^{n+1}(1-8b)^{-1}\,, \tag{35}$$

so that the convergence of K_n to K is geometric.

Moreover, if $B\neq B'$ in (31), but $K=F(K)$ and $K'=F'(K')$, then (31) becomes

$$\begin{aligned}\|K-K'\|&=\|F(K)-F'(K')\|\\&\leqslant\|B-B'\|+8b\,\|K-K'\|\\&\leqslant(1+8b+(8b)^2+\cdots)\|B-B'\|\\&=(1-8b)^{-1}\|B-B'\|\,.\end{aligned} \tag{36}$$

It follows that if B satisfies (26) and if we define $\Theta' B$ as the unique solution of Eq. (25), then $\Theta'\!:B\to T$ is a (nonlinear) mapping continuously defined on the space of *all* backscattering kernels B satisfying (26) with values in the space of all scattering kernels T satisfying (25) and (28). Moreover, if $T=\Theta' B$, then

$$\Theta(\Theta' B)=\Theta T=\Theta B-\Theta(1-\Theta)TT^{*}=B\,, \tag{37}$$

so that Θ is both a left and right inverse for Θ'. Hence Θ' carries the space of backscattering kernels satisfying (26) one-to-one and bicontinuously *into* the space of scattering kernels satisfying (25) and (28) and, by (23), *onto* the subspace of T satisfying (26).

We can now summarize our results as follows.

Theorem: There is a one-to-one bincontinuous (nonlinear) mapping between the space of local potential kernels V satisfying (9) and the space of backscattering kernels B satisfying (26). This mapping is given by the composition of Φ and Θ, with inverse given by the composition of Θ^{-1} and Φ^{-1}. If $\|V\|\leqslant a<1$, then $\|B\|<a(1-a)^{-1}$ by (10) and (23), while if $\|B\|\leqslant b<1/8$, then $\|V\|\leqslant b+4b^2<3/16$ by (24) and (23). If B and B' correspond to V and V', then $\|B-B'\|\leqslant(1-a)^{-2}\|V-V'\|$ by (12), while $\|V-V'\|\leqslant(1+4b)(1-8b)^{-1}\|B-B'\|$ by (17), (36), and (24).

A similar result obtains if instead of the backscatter data we start from fixed-aspect data, i.e., from values of $T(\mathbf{k}',\mathbf{k})$ where $|\mathbf{k}|=|\mathbf{k}'|$ and the ingoing direction $\boldsymbol{\omega}=\mathbf{k}/|\mathbf{k}|$ is fixed, say along the negative x_3 axis. In this case we set

$$2\mathbf{h}=\mathbf{k}'-\mathbf{k}\quad(\mathbf{k}=|\mathbf{k}|\boldsymbol{\omega})\,, \tag{38}$$

and note that as $(\mathbf{k}',\mathbf{k})$ vary through the fixed-aspect values, the vector $\mathbf{h}$ varies through the half space $\mathbf{h}\cdot\boldsymbol{\omega}<0$. Moreover, $\mathbf{h}$ determines the fixed-aspect values of $\mathbf{k}$ and $\mathbf{k}'$ uniquely through the relations

$$|\mathbf{k}|=-|\mathbf{h}|^2/\mathbf{h}\cdot\boldsymbol{\omega}\,, \tag{39}$$

$$\mathbf{k}=|\mathbf{k}|\boldsymbol{\omega}=-(|\mathbf{h}|^2/\mathbf{h}\cdot\boldsymbol{\omega})\boldsymbol{\omega}=\theta\mathbf{h}\,, \tag{40}$$

$$\mathbf{k}'=\mathbf{k}+2\mathbf{h}=2\mathbf{h}-(|\mathbf{h}|^2/\mathbf{h}\cdot\boldsymbol{\omega})\boldsymbol{\omega}=\theta'\mathbf{h}\,. \tag{41}$$

Hence, given the fixed-aspect data for $T(\mathbf{k}',\mathbf{k})$, we may redefine the function B, for $\mathbf{h}\cdot\boldsymbol{\omega}<0$, by setting

$$B(2\mathbf{h})=T(\theta'\mathbf{h},\theta\mathbf{h})=T(\mathbf{k}',\mathbf{k})\quad\text{if }\mathbf{h}\cdot\boldsymbol{\omega}<0\,, \tag{42}$$

with $\mathbf{k}$ and $\mathbf{k}'$ given by (39)–(41). For $\mathbf{h}\cdot\boldsymbol{\omega}>0$, since we want $V(\mathbf{k})=\bar{V}(-\mathbf{k})$, we set

$$B(2\mathbf{h})=\overline{B(-2\mathbf{h})}=\overline{T(\mathbf{k}',\mathbf{k})}\quad\text{if }\mathbf{h}\cdot\boldsymbol{\omega}>0\,. \tag{43}$$

For the plane $\mathbf{h}\cdot\boldsymbol{\omega}=0$, we note that if $\mathbf{h}\cdot\boldsymbol{\omega}\to 0^{+}$ with $|\mathbf{h}|=$ const, then from (39) $|\mathbf{k}|=|\mathbf{k}'|\to\infty$, so $T(\mathbf{k}',\mathbf{k})\to 0$. Hence we set

$$B(2\mathbf{h})=0\quad\text{if }\mathbf{h}\cdot\boldsymbol{\omega}=0\,. \tag{44}$$

Then $B(2\mathbf{h})$ is the function determined by the fixed-aspect data according to (42)–(44) which will play for the case of fixed-aspect data the same role that $B(2\mathbf{h})$ as given by (18) played for the backscatter data.

We must also redefine the projection operation Θ so that (21) still holds with B defined by (42)–(44). This is done by setting $2\mathbf{h}=\mathbf{k}'-\mathbf{k}$, and

$$(\Theta K)(2\mathbf{h})=\begin{cases}K(\theta'\mathbf{h},\theta\mathbf{h}) & \mathbf{h}\cdot\boldsymbol{\omega}<0\,,\\ 0 & \mathbf{h}\cdot\boldsymbol{\omega}=0\,,\\ \overline{K(-\theta'\mathbf{h},-\theta\mathbf{h})} & \mathbf{h}\cdot\boldsymbol{\omega}>0\,.\end{cases} \tag{45}$$

Then we must verify that (20)–(23) still hold for this Θ. With these modifications the proof goes through as before, and we obtain a one-to-one bicontinuous correspondence between the space of local potential kernels and the space of fixed-aspect kernels.

A similar result obtains if instead of fixed-aspect data we start from fixed-scattering-angle data, i.e., from values of $T(\mathbf{k}',\mathbf{k})$ where $|\mathbf{k}|=|\mathbf{k}'|$ and the outgoing direction $\boldsymbol{\omega}'=\mathbf{k}'/|\mathbf{k}'|$ is fixed. This situation is formally similar to the fixed-aspect situation with the roles of $\mathbf{k}$ and $\mathbf{k}'$ interchanged; we shall not insist on the details here.

More generally, we may start from any three-parameter subset of scattering data which can be smoothly parametrized by the difference $2\mathbf{h}=(\mathbf{k}'-\mathbf{k})$, so that for $(\mathbf{k}',\mathbf{k})$ in this subset (with $|\mathbf{k}'|=|\mathbf{k}|$) we may write $(\mathbf{k}',\mathbf{k})=(\theta'\mathbf{h},\theta\mathbf{h})$. Then as $2\mathbf{h}$ runs through $\mathbb{R}^3$, $(\theta'\mathbf{h},\theta\mathbf{h})$ runs through the given subset of $\mathbb{R}^6$, and $B(2\mathbf{h})=T(\theta'\mathbf{h},\theta\mathbf{h})$ runs through the given scattering data. The projection operation Θ is now defined by

$$\Theta K(2\mathbf{h})=K(\theta'\mathbf{h},\theta\mathbf{h})\,, \tag{46}$$

with $2\mathbf{h}=\mathbf{k}'-\mathbf{k}$, and properties (20)–(23) are verified. Then everything goes through as before.

3. REFRACTION SCATTERING

The scattering of a wave function $\varphi(\mathbf{x},\mathbf{k})$ from a variable index of refraction $N(x)$ is governed by the wave equation

$$(\nabla^2+\mathbf{k}^2N(\mathbf{x}))\varphi(\mathbf{x},\mathbf{k})=0,\quad\mathbf{x},\mathbf{k}\in\mathbb{R}\,. \tag{47}$$

If we set $W(\mathbf{x})=1-N(\mathbf{x})$, then (47) becomes

$$(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = \mathbf{k}^2 W(\mathbf{x})\varphi(\mathbf{x},\mathbf{k}) . \tag{48}$$

This equation resembles Eq. (1) with $V(\mathbf{x})$ replaced by $V(\mathbf{x},\mathbf{k}) = \mathbf{k}^2 W(\mathbf{x})$. For fixed $\mathbf{k}$ the behavior of the solutions is identical and the analysis (1)–(6) remains the same. The dependence on $\mathbf{k}$ is different, however, and the subsequent analysis must be adjusted accordingly.

Equation (7) becomes

$$R = W - W\Delta W + W\Delta(W\Delta W) - \cdots , \tag{49}$$

where R, which replaces T, is given by

$$R(\mathbf{k}',\mathbf{k}) = \mathbf{k}^{-2} T(\mathbf{k}',\mathbf{k}) , \tag{50}$$

and Δ, which replaces Γ of Eq. (8), is given by

$$\begin{aligned}\Delta K(\mathbf{k}',\mathbf{k}) &= \mathbf{k}^2(\mathbf{k}'^2 - \mathbf{k}^2 + i0)^{-1} K(\mathbf{k}',\mathbf{k}) \\ &= \mathbf{k}^2 \Gamma K(\mathbf{k}',\mathbf{k}) .\end{aligned} \tag{51}$$

Now if W is small in a suitable Friedrichs norm, for which $\|K\Delta M\| \leqslant \|K\| \|M\|$ (cf. Ref. 4), and

$$\|W\| \leqslant a < 1 , \tag{52}$$

then the series (49) coverges to R, and we have

$$\|R\| \leqslant a(1-a)^{-1} , \tag{53}$$

and

$$\|R - R'\| \leqslant (1-a)^{-2} \|W - W'\| , \tag{54}$$

as before. Moreover, in that case

$$R = W - W\Delta R = WU , \tag{55}$$

where now

$$U = 1 - \Delta R . \tag{56}$$

This operator, unlike that of Eq. (14), is not unitary, and we have no replacement for Eq. (17).

Instead we use Eq. (55), as follows: If we start from the backscatter data, for example, we first set $\mathbf{h} = -\mathbf{k}$ and define the function $B(2\mathbf{h})$ by

$$B(2\mathbf{h}) = R(\mathbf{h}, -\mathbf{h}) = \mathbf{h}^{-2} T(\mathbf{h}, -\mathbf{h}) , \tag{57}$$

and then define the projection operation Θ by (19). We next verify that (20)–(23) hold, with W replacing V and R replacing T. Applying Θ to (55) and solving for W, we get, instead of (24),

$$\begin{aligned} W &= \Theta W = \Theta R + \Theta(W\Delta R) \\ &= B + \Theta(W\Delta R) . \end{aligned} \tag{58}$$

Inserting (58) into (55) we get

$$R = B - (1 - \Theta)W\Delta R . \tag{59}$$

If we combine (58) and (59) into a single equation

$$\begin{pmatrix} W \\ R \end{pmatrix} = \begin{pmatrix} B \\ B \end{pmatrix} - \begin{pmatrix} -\Theta W\Delta R \\ (1-\Theta)W\Delta R \end{pmatrix} , \tag{60}$$

and define the (nonlinear) function $F\binom{V}{K}$ on pairs of kernels $\binom{V}{K}$ according to the formula

$$F\begin{pmatrix} V \\ K \end{pmatrix} = \begin{pmatrix} B \\ B \end{pmatrix} - \begin{pmatrix} -\Theta V\Delta K \\ (1-\Theta)V\Delta K \end{pmatrix} , \tag{61}$$

then we find again, with $\|\binom{V}{K}\| = \max(\|V\|, \|K\|)$, that if

$$\|B\| \leqslant b < 1/8 , \tag{62}$$

and

$$\|\binom{V}{K}\| \leqslant 2b , \tag{63}$$

then

$$\|F\binom{V}{K}\| \leqslant b + 8b^2 , \tag{64}$$

and

$$\|F\binom{V}{K} - F'\binom{V'}{K'}\| \leqslant \|B - B'\| + 8b \|\binom{V-V'}{K-K'}\| . \tag{65}$$

Hence, by the contraction mapping principle, the equation

$$F\binom{V}{K} = \binom{V}{K} , \tag{66}$$

has a unique solution $\binom{V}{K} = \binom{W}{R}$ which determines both W and R uniquely and continuously in terms of B.

This same procedure also works for potential scattering, avoiding the use of T^* at the cost of complicating the iteration procedure described by F.

If we start from other scattering data, then we modify B and Θ accordingly, just as we did for potential scattering.

This same procedure also works for other energy-dependent potentials, so long as the energy dependence can be incorporated into the redefinition of Γ, as in (51).

4. BOUNDARY SCATTERING

The scattering of a wave function $\varphi(\mathbf{x},\mathbf{k})$ from a hard boundary is governed by the wave equation in the exterior of the boundary with a Neumann boundary condition:

$$\begin{aligned} &(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = 0, \quad \mathbf{x}\in D', \quad \mathbf{k}\in\mathbb{R}^3 , \\ &\partial\varphi(\mathbf{x},\mathbf{k}) = 0, \quad \mathbf{x}\in\partial D, \quad \mathbf{k}\in\mathbb{R}^3 . \end{aligned} \tag{67}$$

Here D' is the exterior of a compact region D in $\mathbb{R}^3$ with smooth boundary ∂D, and $\partial\varphi(\mathbf{x},\mathbf{k})$ denotes the exterior normal derivative of $\varphi(\mathbf{x},\mathbf{k})$ at the boundary.

It is well known that the solution $\varphi(\mathbf{x},\mathbf{k})$, which is again to consist of an incoming plane wave plus an outgoing spherical wave, may be expressed in the form (cf. Ref. 8)

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} + 2\int_{\partial D} \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \partial\varphi(\mathbf{y},\mathbf{k})\, d\sigma(\mathbf{y}) . \tag{68}$$

In order to bring this equation into a form which is accessible by our methods, we rewrite it in terms of a volume integral, using the characteristic function of D

$$\chi_D(\mathbf{x}) = \begin{cases} 1 & \mathbf{x}\in D , \\ 0 & \mathbf{x}\in D' , \end{cases} \tag{69}$$

and its gradient, defined, in local coordinates near the boundary, by

$$\nabla\chi_D(\mathbf{x})\, d\mathbf{x} = -\mathbf{n}\delta(r)\, dr\, d\sigma , \tag{70}$$

and vanishing elsewhere. The (68) becomes

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} \int_{\mathbb{R}^3} \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} 2\nabla\chi_D(\mathbf{y})\cdot\nabla\varphi(\mathbf{y},\mathbf{k})\, d\mathbf{y} . \tag{71}$$

Now we can consider (67) as a (singular) special case of the more general problem

$$(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = 2\nabla\chi(\mathbf{x})\cdot\nabla\varphi(\mathbf{x},\mathbf{k}) \quad \mathbf{x},\mathbf{k}\in\mathbb{R}^3 , \tag{72}$$

which also admits a solution of the form (71). Here $\chi(\mathbf{x})$ is a more general potential function, with (69) as a special case. We shall refer to (72) as a form of gradient scattering.

As $|\mathbf{x}|\to\infty$ in (71), we have again

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{e^{i|\mathbf{k}||\mathbf{x}|}}{4\pi|\mathbf{x}|} T(\mathbf{k}',\mathbf{k}) + O\left(\frac{1}{|\mathbf{x}|^2}\right), \tag{73}$$

with $\mathbf{k}' = (|\mathbf{k}|/|\mathbf{x}|)\mathbf{x}$ and

$$T(\mathbf{k}',\mathbf{k}) = \int e^{-i\mathbf{k}'\cdot\mathbf{y}} 2\nabla\chi(\mathbf{y})\cdot\nabla\varphi(\mathbf{y},\mathbf{k})\, d\mathbf{y} . \tag{74}$$

Taking Fourier transforms throughout in (71) and (74), we obtain

$$\varphi(\mathbf{k}',\mathbf{k}) = \delta(\mathbf{k}' - \mathbf{k}) + \int (\mathbf{k}'^2 - \mathbf{k}^2 + i0)^{-1} 2\chi(\mathbf{k}' - \mathbf{k}'') \times(\mathbf{k}' - \mathbf{k}'')\cdot\mathbf{k}''\varphi(\mathbf{k}'',\mathbf{k})\, d\mathbf{k}'' , \tag{75}$$

$$T(\mathbf{k}',\mathbf{k}) = -\int 2\chi(\mathbf{k}' - \mathbf{k}'')(\mathbf{k}' - \mathbf{k}'')\cdot\mathbf{k}''\varphi(\mathbf{k}'',\mathbf{k})\, d\mathbf{k}'' . \tag{76}$$

Inserting (76) into (75), we find

$$\varphi(\mathbf{k}'',\mathbf{k}) = \delta(\mathbf{k}' - \mathbf{k}) - (\mathbf{k}'^2 - \mathbf{k}^2 + i0)^{-1} T(\mathbf{k}',\mathbf{k}) , \tag{77}$$

and inserting (77) into (76), we get

$$T(\mathbf{k}',\mathbf{k}) = -2\chi(\mathbf{k}' - \mathbf{k})(\mathbf{k}' - \mathbf{k})\cdot\mathbf{k} + \int 2\chi(\mathbf{k}' - \mathbf{k}'')(\mathbf{k}' - \mathbf{k}'')\cdot\mathbf{k}'' \times(\mathbf{k}''^2 - \mathbf{k}^2 + i0)^{-1} T(\mathbf{k}'',\mathbf{k})\, d\mathbf{k}'' , \tag{78}$$

or, more formally,

$$\mathbf{R} = \mathbf{W} - \mathbf{W}\cdot\boldsymbol{\Delta}\mathbf{R} . \tag{79}$$

Here we have set

$$\mathbf{R}(\mathbf{k}',\mathbf{k}) = T(\mathbf{k}',\mathbf{k})(-i\mathbf{k}/\mathbf{k}^2) , \tag{80}$$

$$\mathbf{W}(\mathbf{k}' - \mathbf{k}) = 2i\chi(\mathbf{k}' - \mathbf{k})(\mathbf{k}' - \mathbf{k}) = 2(\nabla\chi)(\mathbf{k}' - \mathbf{k}) , \tag{81}$$

and where $\boldsymbol{\Delta}$ is the operation given by

$$\boldsymbol{\Delta}\mathbf{K}(\mathbf{k}',\mathbf{k}) = i\mathbf{k}'(\mathbf{k}'^2 - \mathbf{k}^2 + i0)^{-1}\mathbf{K}(\mathbf{k}',\mathbf{k}) = (\nabla\Gamma)\mathbf{K}(\mathbf{k}',\mathbf{k}) . \tag{82}$$

Now if $\mathbf{W}$ admits a sufficiently small Friedrichs norm,

$$\|\mathbf{W}\| \leqslant a < 1 , \tag{83}$$

then (79) admits an iterative solution of the form (7) for $\mathbf{R}(\mathbf{k}',\mathbf{k})$, and hence for $T(\mathbf{k}',\mathbf{k}) = \mathbf{R}(\mathbf{k}',\mathbf{k})(i\mathbf{k})$, which solves the direct problem for (71).

The difficulty is that if $\mathbf{W} = 2\nabla\chi$, where χ is a characteristic function of the form (69), then $\mathbf{W}(\mathbf{k}' - \mathbf{k})$ dies out too slowly as $|\mathbf{k}|, |\mathbf{k}'| \to \infty$ to admit any useful Friedrichs norm, and so our methods cannot apply directly to (67).

Nevertheless, they do apply to the more general problem (71) for functions $\chi(\mathbf{x})$ which are smooth enough in $\mathbf{x}$ for $\mathbf{W} = \nabla\chi$ to admit a Friedrichs norm satisfying (83).

In that case we can approach the inverse problem just as we did for refractive scattering. Starting from the backscatter data, we form the vector function

$$\mathbf{B}(2\mathbf{h}) = \mathbf{R}(\mathbf{h}, -\mathbf{h}) = T(\mathbf{h}, -\mathbf{h})(i\mathbf{h}/\mathbf{h}^2) , \tag{84}$$

and define the projection operation $\boldsymbol{\Theta}$ by (19). Then we verify that (20)–(23) hold with $\mathbf{W}$ replacing V and $\mathbf{R}$ replacing T. Then we obtain from Eq. (30) the equation

$$\begin{pmatrix} \mathbf{W} \\ \mathbf{R} \end{pmatrix} = \begin{pmatrix} \mathbf{B} \\ \mathbf{B} \end{pmatrix} - \begin{pmatrix} -\boldsymbol{\Theta}\mathbf{W}\cdot\boldsymbol{\Delta}\mathbf{R} \\ (1 - \boldsymbol{\Theta})\mathbf{W}\cdot\boldsymbol{\Delta}\mathbf{R} \end{pmatrix} , \tag{85}$$

just as we obtained (60) from (55). We solve (85) just as we solved (60), obtaining an iterative solution which determines both $\mathbf{W}$ and $\mathbf{R}$ uniquely and continuously in terms of the backscatter kernel $\mathbf{B}$ under the assumption that

$$\|\mathbf{B}\| \leqslant b < 1/8 . \tag{86}$$

The case of fixed-aspect or fixed-scattering-angle data may be treated by a suitable modification of this procedure, as in refractive scattering.

Although our solutions of the direct and inverse problems for (77) fail to give solutions for (67), nevertheless we may hope that further study of (72) may further illuminate the difficulties of (67).

A similar situation obtains in the case of scattering from a soft boundary. Instead of a Neumann boundary condition, we then have a Dirichlet boundary condition:

$$(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = 0 \quad \mathbf{x}\in D' , \ \mathbf{k}\in\mathbb{R}^3 , \qquad \varphi(\mathbf{x},\mathbf{k}) = 0 \quad \mathbf{x}\in\partial D, \ \mathbf{k}\in\mathbb{R}^3 , \tag{87}$$

Then the solution satisfies, instead of (68), the equation[8]

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - 2\int_{\partial D} \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \overleftarrow{\partial}\varphi(\mathbf{y},\mathbf{k})\, d\sigma(\mathbf{y}) . \tag{88}$$

Here $\overleftarrow{\partial}$ denotes the exterior normal derivative of the preceding expression at the boundary. This equation may be rewritten with a volume integral, using χ_D again:

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} + 2\int_{\mathbb{R}^3} \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \times\overleftarrow{\nabla}\cdot\nabla\chi(\mathbf{y})\varphi(\mathbf{y},\mathbf{k})\, d\mathbf{y} . \tag{89}$$

Integrating by parts, we find

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} - 2\int \frac{e^{i|\mathbf{k}||\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \times\vec{\nabla}\cdot(\nabla\chi(\mathbf{y})\varphi(\mathbf{y},\mathbf{k}))\, d\mathbf{y} . \tag{90}$$

Hence we can consider (87) as a special case of

$$(\nabla^2 + \mathbf{k}^2)\varphi(\mathbf{x},\mathbf{k}) = 2\nabla\cdot(\nabla\chi(\mathbf{x})\varphi(\mathbf{x},\mathbf{k})) , \tag{91}$$

another form of gradient scattering.

As $|\mathbf{x}| \to \infty$,

$$\varphi(\mathbf{x},\mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{i|\mathbf{k}||\mathbf{x}|}}{4\pi|\mathbf{x}|} T(\mathbf{k}',\mathbf{k}) + O\left(\frac{1}{|\mathbf{x}|^2}\right), \tag{92}$$

where now

$$T(\mathbf{k}',\mathbf{k}) = \int e^{-i\mathbf{k}'\cdot\mathbf{y}} 2\nabla\cdot(\nabla\chi(\mathbf{y})\varphi(\mathbf{y},\mathbf{k}))\, d\mathbf{y} . \tag{93}$$

Equations (90) and (93) lead to the analog of (78)

$$T(\mathbf{k}',\mathbf{k}) = -2\mathbf{k}'\cdot(\mathbf{k}' - \mathbf{k})\chi(\mathbf{k}' - \mathbf{k}) + \int 2\mathbf{k}'\cdot(\mathbf{k}' - \mathbf{k}'')\chi(\mathbf{k}' - \mathbf{k}'')(\mathbf{k}''^2 - \mathbf{k}^2 + i0)^{-1} \times T(\mathbf{k}'',\mathbf{k})\, d\mathbf{k}'' , \tag{94}$$

which may be written as

$$\mathbf{R} = \mathbf{W} - \mathbf{W}\boldsymbol{\Delta}\cdot\mathbf{R} . \tag{95}$$

Here we have set

$$\mathbf{R}(\mathbf{k}',\mathbf{k}) = (-i\mathbf{k}'/\mathbf{k}'^2)T(\mathbf{k}',\mathbf{k}) , \tag{96}$$

and $\mathbf{W}$ and $\boldsymbol{\Delta}$ are defined by (81) and (82).

Equation (95) yields a solution to the direct problem for (91) under the assumption (83), and leads in turn to Eq. (85), which yields a solution to the inverse problem for (91) under

the assumption (86). As in the case of the hard boundary, none of these solutions can apply to (87), because there χ is not smooth enough to meet the assumption (83).

5. COMMENTS

We have shown that, for scattering from a weak potential or from a weakly inhomogeneous index of refraction, there is a one-to-one bicontinuous correspondence between the potential or refraction index data and the backscattering or fixed-aspect scattering data. This correspondence is nonlinear, but is in all cases implementable in both directions by computable algorithms.

The principal weakness of our result is its restriction to cases where the data are small in norm, i.e., to cases where (9) and (26) or their analogs hold.

This weakness is more than a failure of method, since the result is known to be false for the one-dimensional problems obtained from a partial wave decomposition of the scattering from a radial potential. There it is possible to find a nonzero radial potential for which the l th phase shift is identically zero.[9] This potential is ruled out by our method, because it is strong enough to admit a bound state, and so violates (9).

This weakness rules out completely all problems of potential scattering on the whole one-dimensional line $\mathbb{R}^1$. In that case there are arbitrarily weak potentials which admit bound states. It follows that in this case the Born series (7) cannot converge in norm for any potential. This is because in that case the Green's function in the configuration space representation has the form $\Gamma(x,y) = (e^{i|k||x-y|})/ik$, which is arbitrarily large for small $|k|$. Moreover, in that case the potentials admit no useful Friedrichs norms. The author is indebted to Professor Roger Newton for pointing this out.

Instead of using the Banach contraction mapping principle to solve (32), we can use instead a modified form of Newton's method, due to Kantorovič,[10] which also gives a unique solution under the same hypotheses. The author is indebted to Dr. Louis Rall for pointing this out. A clear discussion of the two methods is given in his MCR report.[11]

Finally we observe that Eq. (17), and hence Eq. (25), holds for *any* potential from our Friedrichs class, whether or not (9) holds, so long as there are no bound states. In the presence of bound states, (15) fails, and hence (17), and the situation becomes much more complicated. In any case it is always possible to obtain Eq. (13), and from it an equation of the form [cf. (61)]

$$\begin{pmatrix} V \\ T \end{pmatrix} = \begin{pmatrix} B \\ B \end{pmatrix} - \begin{pmatrix} -\Theta V\Gamma T \\ (1-\Theta)V\Gamma T \end{pmatrix}, \tag{97}$$

whose solution would solve the inverse problem for potential scattering. The question of the existence and uniqueness of such as solution in general is still wide open. A similar conclusion holds, of course, for the other scattering problems discussed herein.

To end on a positive note, we observe that our results do include the cases originally discussed by Jost and Kohn[2] and their three-dimensional generalization.[1,4] Moreover, we have succeeded in characterizing those scattering kernels which come from weak local potentials, and we hope that this characterization will lead to a better understanding of both the direct and inverse scattering problems

6. CORRECTIONS

We managed to get some signs wrong in parts I and II of this series, and have corrected them in part III. These errors in sign do not in any way affect the validity of our results, but they do effect the final formulas.

Specifically, Eq. (2) in parts I and II should read the same as Eq. (2) in part III. This requires that V be replaced by $-V$ throughout the rest of Sec. 2 in parts I and II. Similarly, Eq. (36) of part II should have the same signs as Eq. (2) of part III; this requires that W be replaced by $-W$ throughout the rest of Sec. 3 in parts I and II.

Finally, Eq. (21) of part I and Eq. (46) of part III are obtained from the Neumann problem for a hard boundary, rather than the Dirichlet problem for a soft boundary. Thus the rest of Sec. 4 of parts I and II apply to hard boundary scattering, rather than soft boundary scattering, as stated. The signs in Eq. (26) of part I and Eq. (51) of part II are still wrong, however; $\nabla\chi$ should be replaced by $-\nabla X$ there and throughout the rest of Sec. 4 in both parts. In all cases the correct sign appears here in part III.

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On the uniqueness of the equilibrium configurations of slowy rotating relativistic fluids [a)]

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We consider the equations of a general relativistic space-time that is stationary, asymptotically Euclidean, diffeomorphic to $\mathbb{R}^4$ and consists of an exterior vacuum solution and an interior perfect fluid in rigid motion. If one requires further that the solution be close to the static spherically symmetric ones (in the sense of a suitable topology on the set of stationary space–time metrics) it is shown that for a given equation of state $\rho(p)$ and given total mass m and (small) angular momentum J there are no smooth curves of physically distinct global axially symmetric solutions. In view of a recent result of Lindblom that all such space-times are axisymmetric this result is quite general. The method is a generalization of the one used to prove (in a "local" sense) the uniqueness of the spherical solution in the static case.

1. INTRODUCTION

In this paper we combine the methods used in Refs. 1 and 2 to prove a "local" uniqueness theorem for global solutions on $\mathbb{R}^4$ of Einstein's field equations for a stationary space-time consisting of a spatially compact interior rigidly rotating perfect fluid and an asymptotically Euclidean vacuum exterior region.

The method of Ref. 2 is based on the work of Cantor[3-5] and Fischer and Marsden[6-7] and less directly, Nirenberg and Walker.[8] Essentially it allows us first to solve the linearized equations only on the spherical background (as was done in Ref. 1), then to conclude that the dimension of the solution space of this linear system on a background close to the spherical one is no greater. Finally we use some global analysis methods to derive from this that the solution of the nonlinear system is unique up to isometries.

The result we have in this last step is not completely satisfactory. Just as in Ref. 2 we are unable to prove that the set X of solutions of the Einstein equations in the selected Banach manifold $\mathscr{P}$ of 3-metrics, scalar and vector potentials on $\mathbb{R}^3$ actually form a submanifold (whose dimension would then be 0 or a small integer, depending on how many parameters are fixed). We can, however, generalize Cantor's slicing theorem to show that $\mathscr{P}$ can locally be written as a product manifold of the orbit of the diffeomorphism group and a transversal manifold $\mathscr{S}$ of physically distinct solutions. We then show that there cannot be in $\mathscr{S}$ a nonconstant differentiable curve of solutions with fixed mass and angular momentum.

This result is analogous to the uniqueness theorem for the Kerr black hole.[9-11] The latter case is somewhat simpler since only the vacuum equations must be solved and leads to a stronger result, namely a unique solution for m and J given in a fairly large range. If there is a (regular) rigidly rotating perfect fluid interior we can expect uniqueness only once the functional form of the equation of state $\rho = \rho(p)$ is fixed, and we can show it only for configurations close enough to the spherical one, i.e. for small angular momentum J. There is little hope to find an upper bound on J for the validity of this result in the general case. (In our approach the use of a proof by contradiction of Nirenberg and Walker precludes this. It undoubtedly exists, however, since we expect branch points as in the classical Maclaurin–Jacobi–ellipsoid series.)

It is worth pointing out that in the classical nonrelativistic theory the uniqueness of the rotating equilibrium configurations cannot be obtained by the same method. Our type of argument would break down at the level of solving the linearized system on the spherical background: The only quantities that do not vanish in this linearized system are related to the "magnetic" part of the gravitational field which is not present int he Newtonian theory. Most discussions of equilibrium configurations of slowly rotating stars in the Newtonian theory start with an assumption about the particular form of the star boundary (ellipsodial or perhaps more complicated.[12] But the classical counterpart of our result (uniquness of a one-parameter series for small J) is found for some special cases in Ref. 13.

In this paper we prove *uniqueness* only, under the condition that

$$0 \leqslant p \leqslant \rho(p) \text{ and } 0 \leqslant d\rho/dp < \infty \ (\rho(p) \text{ piece-wise } C^1) \tag{1.1}$$

and for sufficiently small values of m and J.[14] We do not consider whether to given $\rho(p)$ there exist in fact solutions with $J \neq 0$. We hope to deal with the existence problem later, as well as the related question of isolated distinct solutions with the same $\rho(p)$, m, J in a neighborhood of the spherical one. (We cannot exclude their existence since we do not yet know whether the solution set is a manifold.) Moreover, we also assume that these stationary models are axisymmetric,

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i.e., admit a global one-parameter isometry group whose orbits are closed spacelike curves and which commutes with the timelike isometry group. It has been shown by Lindblom[15] that fluid equilibrium configurations satisfying our conditions are necessarily axisymmetric. His method is similar to Hawking's proof[10] of the stationary black hole theorem and uses analytic extension methods which are somewhat difficult to compare rigorously with our asymptotic conditions. Nevertheless his result shows that we can restrict to the axisymmetric case without a serious loss of generality.

In Sec. 2 we recall the basic equations in the formalism introduced in Refs. 1, 2, and 16, and state the precise assumptions we need. In order to apply as directly as possible the methods of the elliptic theory on noncompact spaces we reformulate these equations in Sec. 3 so as to get a set of second order partial differential equations for as many unknown quantities. It is then fairly straightforward to generalize the methods of Ref. 1 to the stationary case, which we do in Sec. 4.

2. STATIONARY PERFECT FLUID SPACE-TIMES

As in Ref. 1 we consider a globally stationary space-time that is diffeomorphic to a product manifold $\mathbb{R}\times\Sigma$. Einstein's equation for a perfect fluid source,

$$\overset{4}{R}_{\alpha\beta} - (1/\alpha)\overset{4}{R}\,\overset{4}{g}_{\alpha\beta} = \overset{4}{T}_{\alpha\beta} = (\rho + p)\overset{4}{u}_{\alpha}\overset{4}{u}_{\beta} + p\overset{4}{g}_{\alpha\beta}, \tag{2.1}$$

then become in terms of a Riemannian metric γ, a closed 2-form H or its divergence free dual 1-form h and a scalar U on Σ[1],

$$R_{ij} - 2\partial_i U\partial_j U - \tfrac{1}{2}e^{4U}h_i h_j - (\rho + p)e^{-4U}T^2\theta_i\theta_j + [2pe^{-2U} + (\rho + p)e^{-4U}T^2\theta^2]\gamma_{ij} = 0, \tag{2.2}$$

$$\Delta U - \tfrac{1}{2}(\rho + 3p)e^{-2U} + \tfrac{1}{2}e^{4U}h^2 - (\rho + p)e^{-4U}T^2\theta^2 = 0, \tag{2.3}$$

$$\nabla_k(e^{4U}H^{ki}) + 2(\rho + p)e^{-2U}\nu T\theta^i = 0, \tag{2.4}$$

where covariant derivatives refer to γ, R_{ij} is the three-dimensional Ricci tensor, $\theta^2 := \gamma_{ij}\theta^i\theta^j$, $h^i = \tfrac{1}{2}\epsilon^{ijk}H_{jk}$, $h^2 := \gamma^{ij}h_ih_j$, $\nu := (e^{2U} + T^2\theta^2)^{1/2}$ and where θ^i are the components along Σ of the temperature 4-vector ${}^4\theta^\alpha = (1/T)^4u^\alpha$, T being the thermodynamical temperature, mathematically defined up to a constant by the equation

$$(\rho + p)dT = Tdp. \tag{2.5}$$

The thermodynamical equilibrium conditions[1,15] are then equivalent to (2.5),

$$\theta\rfloor H + d(\nu T^{-1}e^{-2U}) = 0 \tag{2.6}$$

and

$$\pounds_\theta U = 0, \quad \pounds_\theta p = 0, \quad \pounds_\theta\gamma = 0. \tag{2.7}$$

We recall that all these quantities (γ, H, U, θ, T) are intrinsically defined on the quotient manifold Σ of the space-time with respect to the trajectories of the global timelike Killing vector field ξ. If local space-time coordinates ($x^0 = t$, x^i) are chosen such that $\xi = \partial_t$ then

$$ds^2 = -e^{2U}(dt + a_idx^i)^2 + e^{-2U}\gamma_{ij}dx^idx^j \tag{2.8}$$

and $H_{ij} = 2\partial_{[i}a_{j]}$. But the quantities a_i do not necessarily define a global 1-form on Σ.

For the time being we adopt the usual regularity assumptions, namely that γ and U be C^1 and piecewise C^3 and h be C^0 and piecewise C^2. For a static solution we can actually assume that γ is C^2 while U has a discontinuous second derivative across the star boundary because ρ drops there discontinously to zero in view of the conditions (1.1). This fact will be significant for technical reasons.[2]

Since we are here only interested in isolated slowly rotating models we can assume that Σ is diffeomorphic to $\mathbb{R}^3$, that the support of ρ and p is compact and that if $r := |x| \to \infty$ then $\gamma_{ij} - \delta_{ij}$ and U are of order $O(1/r)$ and h_i of order $O(1/r^2)$ in terms of some cartesian coordinate system (x^i). These are the usual asymptotic flatness conditions at spacelike infinity,[17] and they are also implied by some more sophisticated definitions (e.g. Geroch[18]) for the special case $\Sigma\simeq\mathbb{R}^3$. We will also assume that the potential U has exactly one critical point, namely a minimum at a point $x_c\in\Sigma$ which we will call the center. This is clearly the case if the situation is nearly spherical since the critical point of U for the spherical solution is a nondegenerate minimum.

The total gravitating mass of an asymptotically flat stationary system is naturally defined by

$$m = (1/4\pi)\int_{\partial D}(\gamma^{jk}\partial_k U + \tfrac{1}{2}e^{4U}H^{ik}\alpha_k)\,d\Sigma_i, \tag{2.9}$$

where D is any domain containing all matter and $\alpha = \alpha_i dx^i$ any 1-form such that $H = d\alpha$, because the value of the integral is independent of the choice of D as well as α (since $\Sigma\simeq\mathbb{R}^3$) and also agrees with the coefficient of $-1/r$ in a asymptotic expansion for the gravitational potential U.

A similar definition for the total angular momentum J is somewhat trickier in the general case. (See, for example, Geroch[18] or Ashtekar and Streubel.[19] However, in the axisymmetric case there exists a formula corresponding to (2.9). Namely, if we define

$$J = (1/16\pi)\int_{\partial D}\{\tfrac{1}{2}H^{ik}(\eta_k + \tfrac{1}{4}e^{4U}\alpha_k\alpha_l\eta^l) + \alpha_k(2\eta^k\gamma^{jl} - \eta^j\gamma^{kl})\partial_l U\}d\Sigma_j, \tag{2.10}$$

where again α is such that $H = d\alpha$ and η is a vector field on Σ satisfying

$$\pounds_\eta\gamma = 0, \quad \pounds_\eta U = 0, \quad \pounds_\eta\alpha = 0, \quad \text{when } \pounds_\eta H = 0, \tag{2.11}$$

which has the asymptotic form

$$\eta = x^1\partial_2 - x^2\partial_1 + O(1/r) \tag{2.12}$$

in terms of cartesian coordinates, then J is again independent of the surface ∂D and the choice of α. (This is best seen in the four-dimensional formalism where

$$16\pi J = \int_{\partial D}\left(\sqrt{-\overset{4}{g}}\right)\overset{4}{\nabla}{}^0\overset{4}{\eta}\delta^{123}_{ijk}dx^j\wedge dx^k = \int_D\left(\sqrt{-\overset{4}{g}}\right)\overset{4}{R}{}^0_\rho\eta^\rho\,dx^1\wedge dx^2\wedge dx^3$$

for a 4-Killing vector field ${}^4\eta$ that commutes with $\xi = \partial_t$ and is everywhere spacelike.)

If, in view of the asymptotic conditions, one writes the cartesian components γ_{ij}, h_i and U in the form

$$\gamma_{ij} = \delta_{ij} + r^{-1}\overset{1}{\gamma}_{ij} + O(r^{-2}), \quad h_i = \overset{1}{h}_i r^{-2} + O(r^{-3}),$$

$$U = \overset{1}{U} r^{-1} + O(r^{-2}),$$

with $x^k \partial_k {}^1\gamma_{ij} = 0$, etc., then the vacuum field equations and (2.9) immediately give that ${}^1U$ is equal to the constant $-m$. It is known that for a stationary and thus nonradiating system the quantities ${}^1\gamma_{ij}$ and ${}^1h_i$ can be made to vanish by a suitable coordinate transformation that is asymptotically Euclidean i.e., consisting of a rotation and a translation). The vanishing of ${}^1\gamma_{ij}$ and ${}^1h_i$ is obtained, for example, by demanding that the coordinates x^i be harmonic (this is essentially the argument given in Ref. 20, p. 456). Not wishing to introduce this coordinate condition we can also derive the result explicitly using the 2 +1–dimensional formalism of Refs. 1 and 16, where U is treated as an intrinsically defined radial coordinate together with the two-dimensional geometry of the surfaces of constant U. It is essential for this argument that these surfaces are topologically 2-spheres.

From now on we will therefore consider the coordinate system of $\Sigma \simeq \mathbb{R}^3$ chosen in such a way that we have

$$\gamma_{ij} = \delta_{ij} + O(r^{-2}), \quad h_i = O(r^{-3}), \quad U = -mr^{-1} + O(r^{-2}). \tag{2.13}$$

Further coordinate transformations that are asymptotically the identity will then not destroy this behavior.

With the asymptotic conditions (2.13) the vacuum field equations imply that

$$h^i = 2Jr^{-3}(\delta^i_3 - 3r^{-2}x^3x^i) + O(r^{-4}) \tag{2.14}$$

provided that also (2.12) holds. A vector potential for this h is then given (up to a gradient) by

$$\alpha_i = 2Jr^{-3}\epsilon_{ik3}x^k + O(r^{-3}). \tag{2.15}$$

3. DESCRIBING THE SET OF EQUILIBRIUM CONFIGURATIONS

The system of Eqs. (2.2)–(2.7) was linearized on the spherical background in Ref. 1 (in a 2 + 1–dimensional formalism). Then, for fixed $\rho(p)$ and m and central value of U, this linearized system was shown to admit only a one-dimensional solution space (after the rotation axis was fixed) that could be thought of as parametrized by the angular momentum. In order to directly extend this result to only nearly spherical background solutions by means of Nirenberg and Walker's[8] and Cantor's[5] theorems we must first modify the equations somewhat so that the linearized system will only consist of as many second-order equations as there are unknown functions. This is not the case for the system (2.2)–(2.7), where, moreover, T and θ are not even defined in the vacuum region.

First, to make Eq. (2.4) of second order, we introduce again the 1-form $\alpha = \alpha_i dx^i$ such that

$$H = d\alpha. \tag{3.1}$$

Since $\Sigma \simeq \mathbb{R}^3$ such a 1-form exists and is determined up to a gradient. It will be unique if we require that

$$\operatorname{div}_\gamma \alpha: \; = \nabla^i \alpha_i = 0 \tag{3.2}$$

and $\alpha_i = O(r^{-2})$ for $r \to \infty$.[21]

In the matter region D we have from (2.6) that $\pounds_\theta \alpha = 0$ for the unique α defined by (3.1) and (3.2). We now can integrate (2.6) and find

$$\theta \lrcorner \alpha - \nu T^{-1} e^{-2U} = -a = \text{const.} \tag{3.3}$$

From (2.7) it follows that θ vanishes at the center, whence $\nu_c = e^{U_c}$ and therefore

$$a = T_c^{-1} e^{-U_c}. \tag{3.4}$$

From (3.3) we find

$$\nu = Te^{2U}(a + \theta \lrcorner \alpha) \tag{3.5}$$

and, solving for T,

$$T^{-2} = e^{2U}(a + \theta \lrcorner \alpha)^2 - e^{-2U}\theta^2. \tag{3.6}$$

The vector field θ is not defined in the vacuum region $\Sigma \setminus D$, but it is an infinitesimal isometry in D. Since it is also tangent to the topological 2-spheres $U = \text{const}$ by (2.7) and vanishes at the center it must have closed orbits and thus represent an infinitesimal rotation.[1] It follows in the axisymmetric case that unless the space-time is spherically symmetric θ must be proportional to the given rotational generator η, i.e.

$$\theta = b\eta, \quad b = \text{const in } D, \tag{3.7}$$

where we assume that η is globally defined on Σ and satisfies (2.11) and (2.12).

Since we assume axial symmetry it might seem reasonable to eliminate an angular variable and work in the (r, θ)–half plane. However, for global arguments this quotient space is not particularly convenient and we could not immediately apply the methods of the next section. Similarly, if we were to consider η as a fixed vector field on Σ when parametrizing the set of equilibrium configurations the structure of the group of diffeomorphisms leaving η invariant would be more complicated. So it seems best to treat η also as a variable. In view of the first of (2.11) it satisfies the second order equation

$$\operatorname{div}_\gamma \circ \pounds_\eta \gamma = \nabla^i(\nabla_i \eta_j + \nabla_j \eta_i) dx^j = 0. \tag{3.8}$$

For the temperature T we have from (2.5) in D

$$T = T_b \cdot \exp \int_0^p \frac{d\bar{p}}{\bar{p} + \rho(\bar{p})}, \tag{3.9}$$

where T_b is the temperature on the surface ∂D of the body, defined by $p = 0$. Since for each different value of T_b of the surface temperature we get an otherwise identical model with the temperature differing at each point of D by a constant factor we are going to keep T_b fixed once and for all.

If the tensor fields γ, U, α, η and the constants a and b are given then our model will be uniquely determined since θ is given by (3.7) in the domain D, T by (3.6) and finally ρ and p as functions on D by (3.9).

We are now ready to describe the set $S_{\rho(p)}$ of (slowly rotating equilibrium) stellar models as follows. For a fixed

manifold Σ (diffeomorphic to $\mathbb{R}^3$ which we consider provided with a fixed coordinate system) let $\mathscr{P}$ to be the set of all sextuples $\sigma = (\gamma, U, \alpha, \eta, a, b)$ satisfying the regularity and asymptotic conditions described above (which will be made more precise in the next section).

Then the set $S_{\rho(p)}$ of stellar models to a given equation of state $\rho = \rho(p)$ [subject to the conditions (1.1)] can be described as the inverse image $\mathscr{L}^{-1}(0) \subset \mathscr{P}$, where $\mathscr{L}$ is the map

$$\mathscr{L}: (\gamma, U, \alpha, \eta, a, b) \to (R_{ij} - 2\partial_i U \partial_j U + \tfrac{1}{2}e^{4U}h_i h_j + (\rho + p)e^{-4U}T^2\theta_i\theta_j + (2pe^{-2U} + (\rho + p)T^2\theta^2 e^{-4U})\gamma_{ij},$$

$$\Delta U - \tfrac{1}{2}(\rho + 3p)e^{-2U} + \tfrac{1}{2}e^{4U}h^2 - (\rho + p)e^{-4U}T^2\theta^2,\ e^{-4U}\nabla^r\nabla_{|r}(\alpha_k e^{4U}) + (\rho + p)e^{-6U}\nu T\theta_k,\ \nabla^r\nabla_{(r}\eta_{k)}), \tag{3.10}$$

where θ, T, ν, p are defined by (3.7), (3.6), (3.5) and (3.9), respectively.

We have chosen this particular map, so as to have as many second order equations as unknown functions. It is clear that the first three components of the equations

$$\mathscr{L}(\sigma) = 0$$

correspond to (2.2), (2.3), and (2.4), respectively, and the last to (3.8). We have not included the stronger Eqs. (2.11) nor the gauge condition (3.2) on α since it will turn out that the chosen equations already determine the equilibrium configuration uniquely up to the two integration constants m and J, arbitrary diffeomorphisms (asymptotic to the identity), and gradient fields added to α.

4. LINEARIZED EQUATIONS ON A NEARLY SPHERICAL BACKGROUND

A. Cantor's weighted Sobolev spaces[3-5]

We recall here only the most basic definitions. A slightly more complete review of those results of Nirenberg and Walker[8] and of Cantor that we use is given in Ref. 2.

Let $p \geqslant 0$ and let $\| \ \|_p$ denote the L^p–norm on the set $C_0^\infty(\mathbb{R}^n, \mathbb{R}^m)$ of C^∞–maps with compact support. Then $M^p_{s,\delta} = M^p_{s,\delta}(\mathbb{R}^n, \mathbb{R}^m)$ is defined to be the completion of C_0^∞ with respect to the norm

$$\|f\|_{p,s,\delta} := \sum_{|\alpha| \leqslant s} \|\sigma(x)^{(|\alpha| + \delta)} D^\delta f\|_p (s \in \mathbb{N},\ \delta \in \mathbb{R}), \tag{4.1}$$

where $\sigma^2(x) := 1 + |x|^2$, $\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}^n$, $|\alpha| := \Sigma\alpha_i$ and $D^\alpha f := \partial^{|\alpha|} f / (\partial x^{\alpha_1} \ldots \partial x^{\alpha_n})$. If $f \in C^\infty(\mathbb{R}^n, \mathbb{R}^m)$ then define

$$M^p_{s,\delta}(f) := \{g: \mathbb{R}^n \to \mathbb{R}^m / (g - f) \in M^p_{s,\delta}\}.$$

For example, if f admits an asymptotic expansion, $f(x) = |x|^{-\alpha} \Sigma_{k=0}^\infty [|x|^{-k} f^k(x)]$ with $x^i \partial_i f^k = 0, f^0 \neq 0$, then $f \in M^p_{s,\delta}$ iff $\alpha > \delta + n/p$.

The inclusion maps $M^p_{s_1,\delta} \to M^p_{s_2,\delta}$ for $s_1 \geqslant s_2$, $M^p_{s,\delta_1} \to M^p_{s,\delta_2}$ for $\delta_1 \geqslant \delta_2$ and $M^p_{s,\delta} \to C^k$ for $\delta \geqslant 0$ and $k + n/p < s$ are continuous.

If $p > 1$, $s > n/p$, $0 \leqslant k \leqslant s$, $\delta, \delta' \geqslant 0$ then any pointwise multiplication $\mathbb{R}^m \times \mathbb{R}^{m'} \to \mathbb{R}^{m''}$ induces continuous maps

$$M^p_{s,\delta}(\mathbb{R}^n, \mathbb{R}^m) + M^p_{s-k,\delta+k}(\mathbb{R}^n, \mathbb{R}^{m'}) \to M^p_{s-k,\delta+k}(\mathbb{R}^n, \mathbb{R}^{m''}), \tag{4.2}$$

$$M^p_{s,\delta}(\mathbb{R}^n, \mathbb{R}^m) + M^p_{s,\delta'}(\mathbb{R}^n, \mathbb{R}^{m'}) \to M^p_{s,\delta+\delta'}(\mathbb{R}^n, \mathbb{R}^{m''}). \tag{4.3}$$

It is easy to see that partial differentiation induces a continuous map

$$\partial_k: M^p_{s,\delta} \to M^p_{s-1,\delta+1}. \tag{4.4}$$

We use $X^p_{s,\delta}$ to represent both vector fields and 1-forms whose (cartesian) components lie in $M^p_{s,\delta}(\mathbb{R}^3, \mathbb{R})$ and $S^p_{s,\delta}$ for symmetric tensors of rank 2.

We will need the following special case of Cantor's isomorphism theorems:

Theroem 4.1: Let $n > k$ and

$$A_\infty = \sum_{\alpha|=k} \bar{a}_\alpha D^\alpha$$

a homogeneous elliptic operator with constant coefficients on $\mathbb{R}^n$ and

$$A = A_\infty + \sum_{\alpha|<k} b_\alpha(x) D^\alpha$$

an elliptic operator.

Then, if $p > n/(n-k)$, $0 \leqslant \delta < n - k - n/p$, $s \geqslant k + n/p$ and $b_\alpha \in M^p_{s-k,k-|\alpha|}$, A maps $M^p_{s,\delta}$ continuously into $M^p_{s-k,\delta+k}$ with closed range and finite-dimensional kernel.

The following is an immediate consequence of a theorem of Nirenberg and Walker.[8]

Theorem 4.2: If $n, k, p, \delta, A_\infty$ and A are as in theorem 4.1 with $b_\alpha(x)$ bounded and $s \geqslant k$ then there exists an $\epsilon > 0$ such that if $A' = A_\infty + \Sigma b'_\alpha(x) D^\alpha$ is another elliptic operator for which

$$\sup_{x \in \mathbb{R}^n} (1 + |x|)^{k-|\alpha|+\delta} |b_\alpha(x) - b'_\alpha(x)| < \epsilon \ (|\alpha| \leqslant k),$$

then the dimension of $\ker A'$ is less than or equal to the dimension of $\ker A$.

B. A Banach manifold of nearly spherical stationary space-times

Suppose again an equation of state subject to the conditions (1.1) as well as the surface temperature T_b is fixed. For every value of m in some interval $(0, m_{\text{crit}})$ there is then a spherically symmetric static model $(\boldsymbol{\gamma}, \mathbf{U})$ which is unique, at least if also the value U_b of the potential U on the star surface is given. In fact, U_b turns out to be determined by m, although this is more difficult to show in general.[2]

We now fix $\boldsymbol{\eta} = \partial_\varphi$ in terms of a polar coordinate system related to the asymptotically cartesian system in the usual way, so that η has the form (2.12) for $r \to \infty$. Since $\theta = 0$ in the static case we have $\mathbf{b} = 0$ and $\mathbf{a} = T_b^{-1} e^{U_b}$ from (3.5). Thus giving $\mathbf{a}$ is equivalent to giving U_b in the static case.

For a given m we denote this so described spherically symmetric solution by $\boldsymbol{\sigma} = (\boldsymbol{\gamma}, \mathbf{U}, \boldsymbol{\alpha} = 0, \boldsymbol{\eta}, \mathbf{a}, \mathbf{b} = 0)$.

For $p > 3$, $\delta \in (0, 1 - 3/p)$ and an integer $s > 2 + 3/p$ define now

$$\tilde{\mathscr{P}}^{p}_{s-1,\delta+1} := \{(h_{ij}, u, \beta_i, \zeta^i, A, B) | h_{ij} = h_{ji}, u, \beta \in M^{p}_{s-1,\delta+1}, \tag{4.5}$$

$$\zeta^i \in M^{p}_{s-1,\delta}, (\gamma_{ij} + h_{ij}) \text{ positive definite}, A, B \in \mathbb{R}\}.$$

Then $\tilde{\mathscr{P}}^{p}_{s-1,\delta+1}$ is an open subset of a Banach space and therefore the set

$$\tilde{\mathscr{P}}^{p}_{s-1,\delta+1} := \{\sigma = (\gamma, U, \alpha, \eta, a, b) / (\gamma - \boldsymbol{\gamma}, \hat{U} - \hat{\mathbf{U}}, \alpha, \eta - \boldsymbol{\eta}, a - \mathbf{a}, b) \in \tilde{\mathscr{P}}^{p}_{s-1,\delta+1}\}, \tag{4.6}$$

which is in one-to-one correspondence with $\mathscr{P}^{p}_{s-1,\delta+1}$ carries a Banach manifold structure. Here $\hat{U}$ and $\hat{\mathbf{U}}$ are related to U and $\mathbf{U}$, respectively, by

$$\hat{U} := U - f_0 p^2 e^{-4U}, \tag{4.7}$$

where f_0 is the value of $1/(4(\rho + 3p)e^{-2U}\gamma^{ij}\partial_i U \partial_j U)$ on the boundary of the spherically symmetric static solution.[22]

According to this definition all solutions σ of Einstein's equations in $\mathscr{P}^{p}_{s-1,\delta+1}$ will have the same total mass m.

C. Action of the diffeomorphism and gauge group

We extend here theorem 3.3 of Ref. 2 which was itself an adaptation of Cantor's slice theorem for the action of a diffeomorphism group on asymptotically Euclidean Riemannian manifolds.

Let

$$\mathscr{D}^{p}_{s,\delta} := \{\varphi \in M^{p}_{s,\delta}(\mathbb{1}) / \varphi^{-1} \text{ exists and } \varphi^{-1} \in M^{p}_{s,\delta}(\mathbb{1})\}, \tag{4.8}$$

where $\mathbb{1}$ is the identity map of $\mathbb{R}^3$. According to Ref. 4 this is an open submanifold of $M^{p}_{s,\delta}(1)$ and a topological group.

Let

$$\mathscr{G}^{p}_{s,\delta} := \mathscr{D}^{p}_{s,\delta} \times M^{p}_{s,\delta}\{(\varphi, \chi) / \varphi \in \mathscr{D}^{p}_{s,\delta},\ \chi \in M^{p}_{s,\delta}(\mathbb{R}^3, \mathbb{R})\}, \tag{4.9}$$

and define

$$A: \mathscr{G}^{p}_{s,\delta} \times \mathscr{P}^{p}_{s,\delta} \to \mathscr{P}^{p}_{s,\delta}: ((\varphi, \chi), (\gamma, U, \alpha, \eta, a, b)) \to (\varphi^*\gamma,\ U \circ \varphi,\ \varphi^* a + d\chi,\ \varphi_*^{-1}\eta,\ a,\ b), \tag{4.10}$$

where φ^* denotes the pull back by the diffeomorphism φ of the appropriate covariant tensor field. Equip $\mathscr{G}^{p}_{s,\delta}$ with the product-differentiable structure. It also carries a group structure as the semidirect product of $\mathscr{D}$ and the abelian group $M^{p}_{s,\delta}$ with respect to the natural action of $\mathscr{D}$ on M by pull backs.

Theorem 4.3: If $p > 3$ and $s > 2 + 3/p$ (and $\delta = 0$) then

(i) A defines a continuous action of $\mathscr{G}^{p}_{s,0}$ on $\mathscr{P}^{p}_{s-1,1}$. $A_{(\varphi,\chi)}: \sigma \to A((\varphi, \chi), \sigma)$ is C^∞ and if $\sigma \in \mathscr{P}^{p}_{s-1+k,1}$, then $A_\sigma : (\varphi, \chi) \to A((\varphi, \chi), \sigma)$ is C^k for $k = 0$ and 1;

(ii) If $\sigma \in \mathscr{P}^{p}_{s-1+k,1}$ (for $k = 0$ or 1), then the orbit $\mathscr{O}_\sigma := \{A((\varphi, \chi), \sigma) / (\varphi, \chi) \in \mathscr{G}^{p}_{s,\delta}\} \subset \mathscr{P}^{p}_{s-1,1}$ is a C^k-submanifold.

(iii) If $\sigma \in \mathscr{P}^{p}_{s,1}$ then there exists a neighborhood V of $(\mathbb{1}, 0)$ in $\mathscr{G}^{p}_{s,0}$ and a slice of the action, i.e. a submanifold $\mathscr{S}$ of $\mathscr{P}^{p}_{s-1,1}$ containing σ such that $((\varphi, \chi), \sigma') \to A((\varphi, \chi), \sigma')$ is a homeomorphism of $V \times \mathscr{S}$ onto a neighborhood U of σ in $\mathscr{P}^{p}_{s-1,1}$ and $\mathscr{O}_\sigma \cap \mathscr{S} = \{\sigma\}$.

Proof:

(i) The proof is analogous to theorem 3.3 of Ref. 2 for γ and $\hat{U}$. Assume first that $\delta \in [0, 1 - 3/p)$ as in that theorem. Since $\chi \to d\chi$ is smooth, $(\varphi, \alpha) \to \varphi^*\alpha_i = \partial\varphi^k/\partial x^i (\alpha \circ \varphi)_k$ is continuous by Theorem 1.2 of Ref. 4 and linear in α, $((\varphi, \chi), \alpha) \to \varphi^*\alpha + d\chi$ is C^∞ in α a continuous in (φ, χ). If $\alpha \in X^{p}_{s,1+\delta}$ then $\partial_k \alpha \in M^{p}_{s-1,\delta}$ and $(\varphi, \partial_k \alpha) \to \varphi^* \partial_k \alpha$ is continuous. For the corresponding proof for $(\varphi, \eta) \to \varphi_*^{-1}\eta$ it is necessary to set $\delta = 0$ to satisfy the condition $\sigma^{|\alpha|-1+\delta} D^\alpha \eta$ is bounded, required in Theorem 1.2 of Ref. 4.

(ii) A_σ is injective since there are no nontrivial isometries in $\mathscr{D}^{p}_{s,\delta}$[5,23] and there are no constants in $M^{p}_{s,\delta}$. If $k = 1$ the tangent map TA_σ at $\varphi = \mathbb{1}$, $\chi = 0$ is given by

$$(\xi, f) \to (\pounds_\xi \gamma,\ \pounds_\xi \hat{U},\ \pounds_\xi \alpha + df,\ \pounds_\epsilon \eta, 0, 0) \in S^{p}_{s-1,1} \oplus M^{p}_{s-1,1} \oplus X^{p}_{s-1,1} \oplus X^{p}_{s-1,0} \oplus \mathbb{R} \oplus \mathbb{R} \approx T_\sigma \mathscr{P}^{p}_{s-1,\delta+1},$$

where $\xi \in X^{p}_{s,0}$. Cantor's version of the Berger–Ebin[24] decomposition, $S^{p}_{s-1,1} = K_\gamma(X^{p}_{s,0}) + J_\gamma$, where $K_\gamma : \xi \to \pounds_\xi \gamma$ and $J_\gamma := \{l \in S^{p}_{s-1,1} \operatorname{div}_\gamma l = 0\}$, together with the splitting[5] $X^{p}_{s-1,1} = d(M^{p}_{s,0}) \oplus \mathscr{J}^{p}_{s-1,1}$, where $\mathscr{J}^{p}_{s-1,1} = \{\omega \in X^{p}_{s-1,1} \operatorname{div}_\gamma \omega = 0\}$ imply that the image of $T_{(1,0)}A_\sigma$ splits, so that A_σ is a C^1-embedding.

(iii) Choose open neighborhoods V of 0 in J_γ and W of 0 in $\mathscr{J}^{p}_{s-1,1}$ such that $\gamma + l$ is positive definite for $l \in V$. Then, if $\sigma \in \mathscr{P}^{p}_{s,1}$, $\mathscr{S} = \{(\gamma + 1, \hat{U} + u, \alpha + \beta, \eta + \zeta, a + A, b + B) | l \in V, u \in M^{p}_{s-1,1}, \beta \in W, \zeta \in X^{p}_{s-1,0}, A, B \in \mathbb{R}\}$ is clearly an embedded submanifold of $\mathscr{P}^{p}_{s-1,1}$. The homeomorphism is obtained by use of the decomposition theorems as in Ref. 2.

D. Solution of the linearized Einstein equations

We conjecture that the set of solutions of Einstein's equations in some neighborhood V of $\boldsymbol{\sigma}$ in $\mathscr{P}^{p}_{s-1,1}$, namely $\mathscr{L}^{-1}(O) \cap V$, is equal to

$$\bigcup_{\sigma \in \mathscr{C}} \mathscr{O}_\sigma \cap V,$$

where $\mathscr{C}$ is a one-dimensional submanifold of $\mathscr{P}^{p}_{s-1,1}$ passing through $\boldsymbol{\sigma}$ and parametrized by the angular momentum. As in the static case, however, $\mathscr{L}' = T_\sigma \mathscr{L}$ at $\sigma = \boldsymbol{\sigma}$ is not surjective and we cannot show transversality of $\mathscr{L}$ over a suitable submanifold of the image space of $\mathscr{L}$ and so are unable to show that $\mathscr{L}^{-1}(0)$ is a submanifold. But since, in a neighborhood of $\boldsymbol{\sigma}$, the set of equivalence classes of $\mathscr{P}^{p}_{s-1,1}$ with respect to the action of $\mathscr{G}^{p}_{s,0}$ is in one-to-one correspondence with the slice $\mathscr{S}$ through $\boldsymbol{\sigma}$ we show that there can be no nonconstant C^1-curve in $\mathscr{S} \cap S_{\rho(p)}$ passing through a particular solution (existence assumed) with some angular momentum unless the curve passes through solutions with different angular momenta.

Let $(c = \delta\gamma, u = \delta U, \beta = \delta\alpha, \zeta = \delta\eta, A = \delta a, B = \delta b) \in T_\sigma \mathscr{P}^{p}_{2,1}$. For $\sigma = \boldsymbol{\sigma} \in \mathscr{P}^{p}_{s,1}$ we have from the proof of Theorem 4.3 the decomposition

$$C = \pounds_\xi \gamma + \Phi, \quad \operatorname{div}_\gamma(\Phi) = 0, \tag{4.11}$$

$$u = \pounds_\xi U + \Psi, \tag{4.12}$$

$$\beta = \pounds_\xi \alpha + df + \omega, \quad \operatorname{div}_\gamma(\omega) = 0, \tag{4.13}$$

$$\zeta = \pounds_\xi \eta + \nu, \tag{4.14}$$

where $\xi\in X^p_{3,0}$, $\Phi\in S^p_{2,1}$, $\Psi\in M^p_{2,1}$, $\omega\in X^p_{2,1}$, $f\in M^p_{3,0}$, $\nu\in X^p_{2,0}$ are all unique. A standard calculation gives that

$$\mathscr{L}'(\sigma)\colon\ T_\sigma \mathscr{P}^p_{2,1}\to S^p_{0,3}\oplus M^p_{0,3}\oplus X^p_{0,3}\oplus X^p_{0,2} =: \hat{Y} \tag{4.15}$$

is given by

$$\begin{aligned}\mathscr{L}'_1(\sigma)(c,u,\beta,\zeta,A,B)_{ij} &= \tfrac{1}{2}\nabla^r\nabla_r c_{ij} + \tfrac{1}{2}\nabla_i\nabla_j c^r_r - \nabla_{(i}(\nabla^r c_{j)r}) + \big[-3R^r{}_{(i}\delta^s_{j)} + R^{rs}\gamma_{ij} + \tfrac{1}{2}R\delta^r_i\delta^s_j\\ &+ (R_{ij} - \tfrac{1}{2}R\gamma_{ij} - \tfrac{1}{2}h_ih_je^{4U})\gamma^{rs} + e^{4U}h^rh_{(i}\delta^s_{j)} + 2(\rho+p)e^{-4U}T^2\theta^r\theta_{(i}\delta^s_{j)}\\ &- 2pe^{-2U}\delta^r_i\delta^s_j - (\rho+p)T^2\theta^2e^{-4U}\delta^r_i\delta^s_j - \tfrac{1}{2}e^{-6U}(\rho+p)T^2\theta^r\theta^s(4e^{2U}\gamma_{ij}\\ &+ T^2(\rho'+3)(\theta^2\gamma_{ij}-\theta_i\theta_j))\big]c_{rs} + 4\partial_{(i}U\partial_{j)}u \div \big[2h_ih_je^{4U} + 2(\rho+3p)e^{-2U}\gamma_{ij}\\ &+ (\rho+p)e^{-4U}T^2(8\theta^2\gamma_{ij} - 4\theta_i\theta_j + \tau(\rho'+3)(\theta^2\gamma_{ij}-\theta_i\theta_j))\big]u + h_{(i}\epsilon_{j)}{}^{rs}e^{4U}\nabla_r\beta_s\\ &+ \nu T(\rho+p)e^{-4U}\big[2e^{2U}\gamma_{ij} + T^2(\rho'+3)(\theta^2\gamma_{ij}-\theta_i\theta_j)\big]\theta^r\beta_r + (\rho+p)e^{-4U}T^2\big[2\gamma_{k(i}\theta_{j)}\\ &+ 2(\nu T^{-1}e^{2U}\alpha_k - 2\theta_k)\gamma_{ij} + (\rho'+3)(\nu T\alpha_k - T^2e^{-2U}\theta_k)(\theta^2\gamma_{ij}-\theta_i\theta_j)\big](B\eta^k + b\zeta^k)\\ &+ \nu T^2e^{-4U}(\rho+p)\big[2e^{2U}T^{-1}\gamma_{ij} + (\rho'+3)T(\theta^2\gamma_{ij}-\theta_i\theta_j)\big]A,\end{aligned} \tag{4.16}$$

$$\begin{aligned}\mathscr{L}'_2(\sigma)(c,u,\zeta,\beta,A,B) &= \Delta u + \big[2h^2e^{4U} + (\rho+3p)e^{-2U} + (\rho+p)e^{-2U}(4T^2\theta^2e^{-2U} + \tfrac{1}{2}(\rho'+3)\tau^2)\big]u\\ &- \nabla^rU(\nabla^sc_{sr} - \tfrac{1}{2}\nabla_rc^s_s) + \big[\tfrac{1}{2}h^rh^se^{4U} - \nabla^r\nabla^sU - \tfrac{1}{2}h^2\gamma^{rs}\\ &- (\rho+p)T^2e^{-4U}(1+\tfrac{1}{4}(\rho'+3)\tau)\theta^r\theta^s\big]c_{rs} + H^{rs}e^{4U}\nabla_r\beta_s\\ &+ \tfrac{1}{2}(\rho+p)(\rho'+3)\tau T\nu e^{-2U}\theta^r\beta_r + (\rho+p)e^{-2U}T\big[-2Te^{-2U}\theta_r + \tfrac{1}{2}(\rho'+3)\\ &\times(\nu\alpha_r - e^{-2U}T\theta_r)\tau\big]\cdot(\beta\eta^r + b\zeta^r) + \tfrac{1}{2}(\rho+p)(\rho'+3)T\nu\tau e^{-2U}A,\end{aligned} \tag{4.17}$$

$$\begin{aligned}\mathscr{L}'_3(\sigma)(c,u,\beta,\zeta,A,B)_i &= \tfrac{1}{2}\nabla^r\nabla_r\beta_i - \tfrac{1}{2}\nabla_i(\nabla^r\beta_r) + 4\nabla^rU\nabla_{[r}\beta_{i]}\\ &- \big[\tfrac{1}{2}R^r_i + (\rho+p)e^{-6U}T^2(\nu^2(\rho'+3) - e^{2U})\theta_i\theta^r\big]\beta_r\\ &- \big[H^{(k}_i\gamma^{r)s} + \tfrac{1}{2}H^{kr}\delta^s_i\big]\nabla_kc_{rs}\\ &+ \big[-\tfrac{1}{2}e^{-4U}\nabla^r(H^s{}_ie^{4U}) + (\rho+p)\nu Te^{-6U}(\delta^r_i\theta^s + \tfrac{1}{2}e^{-2U}(\rho'+3)T^2\theta^r\theta^s\theta_i)\big]c_{rs}\\ &- 2H^r_i\partial_ru - (\rho+p)\nu Te^{-6U}(4+\tau(\rho'+3)\theta_iu\\ &+ (\rho+p)e^{-6U}T^2\big[\nu T^{-1}\gamma_{ir} + e^{2U}\alpha_r\theta_i + \nu(\rho'+3)(Te^{-2U}\theta_r - \nu\alpha_r)\theta_i\big]\cdot(B\eta^r + b\zeta^r)\\ &- (\rho+p)e^{-6U}T^2((\rho'+3)\nu^2 - e^{2U})\theta_iA,\end{aligned} \tag{4.18}$$

$$\begin{aligned}\mathscr{L}'_4(\sigma)(c,u,\beta,\zeta,A,B)_i &= \nabla^r\nabla_{(r}\zeta_{i)} + \tfrac{1}{2}\eta^r\nabla_r(\nabla_sc^s_i) - \tfrac{1}{2}\nabla^r\eta_i(\nabla_sc^s_r) + \nabla^{(r}\eta^{s)}(\nabla_rc_{si} - \tfrac{1}{2}\nabla_ic_{rs})\\ &+ \tfrac{1}{4}(\nabla_i\eta^r + \nabla^r\eta_i)\nabla_rc^s_s + (\tfrac{1}{2}\nabla^s\nabla_s\eta^r + \tfrac{1}{2}R^r{}_s\eta^s)c_{ir} - \tfrac{1}{2}(\nabla^r\nabla^s\eta_i + R^r{}_i{}^s{}_l\eta^l)c_{rs},\end{aligned} \tag{4.19}$$

where $\rho' := d\rho/dp$ and $\tau := 1 + 2e^{-2U}T^2\theta^2$.

$\mathscr{L}'(\sigma)$ is not elliptic but by restricting

$$\mathscr{L}'(\sigma)(c,u,\beta,\zeta,A,B) = 0 \tag{4.20}$$

to the slice $\mathscr{S}$ we can obtain an elliptic operator to which we will be able to apply Theorem 4.2. To this end define [for $x := (c,u,\beta,\zeta)$]

$$\begin{aligned}A_1(\sigma)(x)_{ij} &:= \mathscr{L}'_1(\sigma)(c,u,\beta,\zeta,A,B)_{ij} + \tfrac{1}{2}(K_\gamma\circ\mathrm{div}_\gamma c)_{ij}\\ &- \nu T^2e^{-4U}(\rho+p)\big[2e^{2U}T^{-1}\gamma_{ij}\\ &+ (\rho'+3)T(\theta^2\gamma_{ij}-\theta_i\theta_j)\big]A - (\rho+p)\\ &\times e^{-4U}T^2\big[2\gamma_{k(i}\theta_{j)} + 2(\nu T^{-1}e^{2U}\alpha_k - 2\theta_k)\gamma_{ij}\\ &+ (\rho'+3)(\nu T\alpha_k - T^2e^{-2U}\theta_k)\\ &\times(\theta^2\gamma_{ij}-\theta_i\theta_j)\big]\eta^kB,\end{aligned} \tag{4.21}$$

$$\begin{aligned}A_2(\sigma)(x) &:= \mathscr{L}'_2(\sigma)(c,u,\beta,\zeta,A,B) + \nabla^rU(\mathrm{div}_\gamma c)_r\\ &- \tfrac{1}{2}(\rho+p)(\rho'+3)T\nu\tau e^{-2U}A\\ &- (\rho+p)e^{-2U}T\big[-2Te^{-2U}\theta_r\\ &+ \tfrac{1}{2}(\rho'+3)(\nu\alpha_r - e^{-2U}T\theta_r)\tau\big]\eta^rB,\end{aligned} \tag{4.22}$$

$$\begin{aligned}A_3(\sigma)(x)_i &:= \mathscr{L}'_3(\sigma)(c,u,\beta,\zeta,A,B)_i + \tfrac{1}{2}\partial_i(\mathrm{div}_\gamma\beta)\\ &+ (\rho+p)e^{-6U}T^2[(\rho'+3)\nu^2 - e^{2U}]\theta_iA\\ &- (\rho+p)e^{-6U}T^2\big[\nu T^{-1}\gamma_{ir} + e^{2U}\alpha_r\theta_i\\ &+ \nu(\rho'+3)(Te^{-2U}\theta_r - \nu\alpha_r)\theta_i\big]\cdot\eta^rB,\end{aligned} \tag{4.23}$$

$$A_4(\sigma)(x)_i := \mathscr{L}'_4(\sigma)(c,u,\beta,\zeta,A,B)_i - \tfrac{1}{2}\eta^r\nabla_r(\mathrm{div}_\gamma c)_i. \tag{4.24}$$

It is easy to verify that $A(\sigma) = (A_1, A_2, A_3, A_4)(\sigma)$ is a second order elliptic operator. Equation (4.20) is now equivalent to

$$A_1(\sigma)(x) - \tfrac{1}{2}K_\gamma\circ\mathrm{div}_\gamma c = b_1(\sigma)(A,B)^T, \tag{4.25}$$

$$A_2(\sigma)(x) - \nabla U\lrcorner\mathrm{div}_\gamma c = b_2(\sigma)(A,B)^T, \tag{4.26}$$

$$A_3(\sigma)(x) - \tfrac{1}{2}d(\mathrm{div}_\gamma\beta) = b_3(\sigma)(A, B)^T, \tag{4.27}$$

$$A_4(\sigma)(x) + \tfrac{1}{2}\eta \lrcorner d(\mathrm{div}_\gamma c) = b_4(\sigma)(A, B)^T, \tag{4.28}$$

where the $b_i(\sigma)$ are the obvious row matrices of tensor fields obtained from Eqs. (4.21)–(4.25) [$b_4 = (0, 0)$]. We also write $b(\sigma)$ for $[b_1(\sigma), b_2(\sigma), b_3(\sigma), b_4(\sigma)]$.

We will show that for $\sigma \in \mathscr{S}$ near $\boldsymbol{\sigma}$ and $x = (c, u, \beta, \zeta) \in S^p_{2,1} \oplus M^p_{2,1} \oplus X^p_{2,1} \oplus X^p_{2,0}$ the inhomogeneous equation

$$A(\sigma)(x) = b(\sigma)(A, B)^T \tag{4.29}$$

implies that $c = u = \beta = \zeta = A = B = 0$ if also the variation δJ of the angular momentum corresponding to $(c, u, \beta, \zeta, A, B)$ vanishes.

This will then imply that the solution of (4.20) vanishes if $(c, u, \beta, \zeta, A, B)$ is tangent to the slice and the corresponding $\delta J = 0$.

We will solve (4.29) first on the spherical background $\boldsymbol{\sigma}$ and then extend the result using theorems 4.1 and 4.2.

On the spherical background Eq. (4.29) decouples into

$$A_{1,2}(\boldsymbol{\sigma})(c, u) = b_{1,2}(\boldsymbol{\sigma})(A, 0)^T, \tag{4.30}$$

$$A_3(\boldsymbol{\sigma})(\beta) = b_3(\boldsymbol{\sigma})(0, B)^T, \tag{4.31}$$

$$A_4(\boldsymbol{\sigma})(c, \zeta) = 0, \tag{4.32}$$

where (4.30) is the set of equations obtained in the static case.[25] The analysis there gives us that c, u, ξ, and A vanish. Putting $c = 0$ in (4.32) yields the equation $\mathrm{div}_\gamma \circ K_\gamma \zeta = 0$ which implies $\zeta = 0$ since $\mathrm{div}_\gamma \circ K_\gamma : X^p_{s,0} \to X^p_{s-2}$, is an isomorphism.[26] Letting $K^i = \epsilon^{ijk}\partial_j\beta_k$ Eq. (4.31) becomes

$$\epsilon^{ijk}\partial_j(e^{4U}K_k) = 2(\rho + p)e^{-4U}T^2 aB\eta^i, \tag{4.33}$$

which in the 2 +1–dimensional formalism[27] becomes Eqs. (4.8) and (4.9) of Ref. 1, while $\nabla_i K^i = 0$ becomes (4.11) of Ref. 1. The analysis of these equations shows that for a given B there exists a unique solution K^i which is asymptotically $O(r^{-3})$ at infinity and vanishes if $B = 0$.

Since $T_\sigma \mathscr{P}^p_{2,1}$ splits, i.e., $T_\sigma \mathscr{P}^p_{2,1} = T_\sigma \mathscr{O}_\sigma \oplus T_\sigma \mathscr{S}$ we can investigate the solution β on the two subspaces separately. Since $\beta = \mathscr{L}_\xi \alpha + df$ on $T_\sigma \mathscr{O}_\sigma$ for some $\xi \in X^p_{3,0}$, $f \in M^p_{3,0}$, and $\mathscr{L}(A_{(\varphi,X)}(\boldsymbol{\sigma})) = \varphi^*(\mathscr{L}(\boldsymbol{\sigma}))$ (4.27) implies $d(\mathrm{div}_\gamma df) = 0$, whence $f = 0$ since $\Delta : M^p_{s,0} \to M^p_{s-2,2}$ is an isomorphism. On $T_\sigma \mathscr{S}$ we have $\mathrm{div}_\gamma \beta = 0$ so that β is uniquely determined by K_i and hence by B, and has an asymptotic expansion of $O(r^{-2})$ at infinity and vanishes if $B = 0$. This follows since $K = 0$ implies $\mathrm{div}_\gamma \circ K_\gamma \beta = 0$.

It is easily calculated that the variation of the angular momentum J is given by

$$\delta J = \frac{1}{16\pi} \lim_{r\to\infty} \int_{r = \text{const}} \partial_{[i}\beta_{j]}\eta^j \gamma^{il}\, d\Sigma_l, \tag{4.34}$$

and so will not vanish unless $\beta = B = 0$ [i.e.,: K^i has an asymptotic expansion like (2.14) with J replaced by δJ.] Summarizing we have

Theorem 4.4: The operator equations

$$A(\boldsymbol{\sigma})(c, u, \beta, \zeta) = b(\sigma)(A, B)^T,$$

with $(c, u, \beta, \zeta, A, B) \in T_\sigma \mathscr{P}^p_{2,1}$ imply that c, u, ζ, A vanish and β, B are uniquely determined by δJ, vanishing if $\delta J = 0$.

E. Curves of solutions in $\mathscr{S}$

The presence of the inhomogeneous terms $b(\sigma)(A, B)^T$ does not allow a direct application of theorem 4.2 so we proceed analogously to the static case[2] with the slight complication introduced by having two constants A and B. From Theorem 4.1 it is easily verified that for $\sigma \in \mathscr{P}^p_{3,1}$ (in particular, for $\boldsymbol{\sigma}$) the map

$$A(\sigma): X := S^p_{2,0} \oplus M^p_{2,0} \oplus X^p_{2,0} \oplus X^p_{2,0} \to S^p_{0,2} \oplus M^p_{0,2} \oplus X^p_{0,2} \oplus X^p_{0,2} =: Y$$

is a continuous linear operator with finite-dimensional kernel and closed range.

As in Ref. 2 (4.30) determines c and u uniquely in terms of δm for $x \in X$ while (4.31) determines $\beta \in X^p_{2,0}$ uniquely in terms of δJ and (4.32) determines ζ uniquely in terms of c, as seen above. Thus the solution space of $A(\boldsymbol{\sigma})x - b(\boldsymbol{\sigma})(A, B)^T = 0$ in $X \oplus \mathbb{R} \oplus \mathbb{R} = \{(x, A, B)\}$ is two-dimensional and spanned by $(x_0, 0, B_0)$ and $(y_0, A_0, 0)$ corresponding to the solutions with $(\delta m, \delta J) = (0, J)$ and $(m, 0)$ respectively.

For $\sigma = \boldsymbol{\sigma}$, putting $A = 0$ means $\delta m = 0$ so c and u vanish, as well as ζ by (4.32). Putting $B = 0$ gives $\beta = 0$. The operators $A(\boldsymbol{\sigma})$ and $A(\sigma)$ satisfy the hypothesis of Theorem 4.2, so for σ in a neighborhood of $\boldsymbol{\sigma}$ in $\mathscr{P}^p_{2,1}$ the operator $A(\sigma): X \to Y$ is injective.

Thus there are unique $x_0, y_0 \in X$ such that

$$A(\boldsymbol{\sigma})x_0 = b(\boldsymbol{\sigma})(0, 1)^T, \tag{4.35}$$

$$A(\boldsymbol{\sigma})y_0 = b(\boldsymbol{\sigma})(1, 0)^T. \tag{4.36}$$

In fact $x_0 = (0, 0, \beta_0, 0)$ where $\beta_0 = O(r^{-2})$ at infinity while $y_0 \in X \setminus \hat{X}$, where $\hat{X} := S^p_{2,1} \oplus M^p_{2,1} \oplus X^p_{2,1} \oplus X^p_{2,0}$ is a subspace of faster fall off. Suppose σ is in a neighborhood of $\boldsymbol{\sigma}$ such that

$$\|A(\sigma) - A(\boldsymbol{\sigma})\| < \epsilon_1 \quad \text{and} \quad \|b(\sigma) - b(\boldsymbol{\sigma})\| < \epsilon_2, \tag{4.37}$$

for some small $\epsilon_1, \epsilon_2 > 0$. Then by Theorem 4.2 $\ker_X A(\sigma) = \{0\}$ and there are unique solutions $x, y, \in X$ of

$$A(\sigma)x = b(\sigma)(0, 1)^T \tag{4.38}$$

and

$$A(\sigma)y = b(\sigma)(1, 0)^T. \tag{4.39}$$

Using the fact that $A(\boldsymbol{\sigma}): X \to Y$ is injective and has a closed range and so has a bounded inverse we can show, as in Ref. 2, that x is arbitrarily close to x_0 and y is arbitrarily close to y_0 for small enough ϵ_1 and ϵ_2. Therefore y cannot lie in X and $x = (c, u, \beta, \zeta)$ must have $\beta = 0(|x|^{-2})$ at infinity and thus corresponds to a solution with $\delta J \neq 0$.

By the remark below (4.29) we have:

Theorem 4.5: If $c: [0, 1] \to \mathscr{S} \cap S_{\rho(p)}$ is a C^1–curve of solutions all having the same (small) angular momentum J then c is constant if the slice $\mathscr{S}$ is contained in a small enough neighborhood of $\boldsymbol{\sigma}$.

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Properties of the noise-induced "spurious" drift. I

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The coefficients of Fokker–Planck equations associated to Langevin equations (LE) may be interrelated, since both the diffusion matrix **D** and the noise-induced drift **a** are derived from the same coefficients of the LE. If **D** is regular and if furthermore its dimension M equals the number of independent noise sources (conditions to be dropped in the subsequent paper II), **a** is uniquely determined by **D** if $M = 1$ and independent of **D** if $M \geqslant 3$. For $M = 2$, **a** splits into a nontensor part which is uniquely determined by **D** and a vector field with given divergence. The result for $M \geqslant 3$ means that to any LE with noise terms specified by their covariance matrix only, there exists another stochastically equivalent LE with a fully arbitrary deterministic part. As a byproduct it is shown that any given **a** can be removed by a nonlinear change of the state variables.

1. INTRODUCTION

We consider a physical system obeying the equations of motion

$$\dot{x}^\nu = f^\nu(\mathbf{x}, t) \quad (\nu = 1, ..., N) \tag{1.1}$$

and assume that it is perturbed by M ($\leqslant N$) independent noise sources ξ_i (Gaussian white noise) in such a way that (1.1) becomes

$$\dot{x}^\nu = f^\nu(\mathbf{x}, t) + b_i^\nu(\mathbf{x}, t)\xi_i. \tag{1.2}$$

Summation over double indices is always understood. Equation (1.2) is called a Langevin equation (LE) or a stochastic differential equation (SDE). Its integral form (omitting the symbols of integration) is

$$dx^\nu(t) = f^\nu(\mathbf{x}(t), t)dt + b_i^\nu(\mathbf{x}(t), t)dW_i(t), \tag{1.2'}$$

the $W_i(t)$ being Wiener processes. It is well known[1–6] that stochastic integrals and hence also SDE's are not uniquely defined due to the unbounded variation of the Wiener processes. Here we adopt their "Stratonovich sense" because

(i) the LE is then covariant with respect to nonlinear transformations of the state variables $\mathbf{x}$,[4–6]

(ii) an equation with broadband instead of white noise (more realistic physically) is then reasonably approximated by (1.2).[1,2]

The probability density of the solutions $\{\mathbf{x}(t)\}$ is determined by the Fokker–Planck equation (FPE)[1,2]

$$\partial_t p = -\partial_\nu(F^\nu p) + \tfrac{1}{2}\partial_\mu\partial_\nu(D^{\mu\nu}p), \tag{1.3}$$

where

$$\partial_t = \partial/\partial t, \quad \partial_\nu = \partial/\partial x^\nu,$$

$$F^\nu = f^\nu + a^\nu, \quad a^\nu = \tfrac{1}{2}b_j^\mu\partial_\mu b_j^\nu, \quad D^{\mu\nu} = b_j^\mu b_j^\nu \tag{1.4}$$

and $p(\mathbf{x}, t, \mathbf{x}_0, t_0)d\mathbf{x}$
$= \text{Prob}(\mathbf{x} < \mathbf{x}(t) \leqslant \mathbf{x} + d\mathbf{x} | \mathbf{x}(t_0) = \mathbf{x}_0) \quad (t > t_0)$.

The term a^ν originates from the choice of the Stratonovich sense. In the literature it is called "spurious drift"; we prefer "noise-induced drift" (NID), since it is part of the total drift F^ν observable in an experiment.

Depending on the particular problem it may be more convenient to specify the noise influence directly by the pertinent terms in the FPE, viz. **a** and **D**, instead of the noise coefficients b_i^ν of the LE. Due to the symmetry $D^{\mu\nu} = D^{\nu\mu}$ this requires not more than $M + M(M+1)/2$ functions, compared to the M^2 noise coefficients of the LE. (Different LE's belonging to the same FPE are stochastically—and hence physically—equivalent.) However the a^ν and $D^{\mu\nu}$ are not necessarily independent of each other, since there must exist a set of coefficients b_j^ν such that (1.4) holds. In particular, for $M = 1$, a^1 is even uniquely determined by D^{11}:

$$a^1 = \tfrac{1}{4}\partial_1 D^{11}. \tag{1.5}$$

The purpose of this paper is to investigate this intrinsic connection between a^ν and $D^{\mu\nu}$. More specifically, we will answer the question: which is the set of all NID's a^ν compatible with given diffusion coefficients $D^{\mu\nu}$?

The solution to this problem is relatively simple, if the diffusion matrix $\mathbf{D} = \|D^{\mu\nu}\|$ is regular and if its dimension equals the number M of noise sources. The more general case will be discussed in a second paper. This second part will also include conditions, under which the present situation can be established by a change of variables and by use of stochastic equivalence.

2. THE SET OF POSSIBLE NOISE COEFFICIENTS

In what follows we assume $M \geqslant 2$ and that the variables x^ν which are directly perturbed, have indices $\nu = 1, ..., M$. The remaining variables ($\nu = M + 1, ..., N$) may be considered as parameters, and summations can be restricted to $1 \leqslant \nu \leqslant M$.

We first have to construct all sets of noise coefficients b_i^ν compatible with given diffusion coefficients $D^{\mu\nu}$. For this the matrix notation is convenient. With $\|b_i^\nu\| = \mathbf{B}$ Eqs. (1.4) read

$$\mathbf{D} = \mathbf{B}^T\mathbf{B}, \tag{2.1}$$

$$2a^\nu = (\mathbf{B}^T\partial_\mu\mathbf{B})^{\mu\nu}. \tag{2.2}$$

A possible solution for **B** of Eq. (2.1) is the symmetric positive square root of **D**, and further solutions are obtained by

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multiplication with arbitrary orthogonal matrices $\mathbf{O}(\mathbf{x}, t)$ from the left

$$\mathbf{B} = \mathbf{O}\sqrt{\mathbf{D}}, \tag{2.3}$$

since $\sqrt{\mathbf{D}}\mathbf{O}^T\mathbf{O}\sqrt{\mathbf{D}} \equiv \mathbf{D}$. In fact every solution has this form, as follows from the polar decomposition theorem. Inserting (2.3) into (2.2) gives

$$2a^\nu = (\sqrt{\mathbf{D}}\partial_\mu\sqrt{\mathbf{D}})^{\mu\nu} + (\sqrt{\mathbf{D}}\mathbf{O}^T(\partial_\mu\mathbf{O})\sqrt{\mathbf{D}})^{\mu\nu}. \tag{2.4}$$

While the first term depends on $\mathbf{D}$ alone, the second involves $\mathbf{O}$ also. Thus the NID is not uniquely determined by $\mathbf{D}$. A constant $\mathbf{O}$ however leaves the NID and thus the whole FPE unchanged.

3. RESULTS FOR CONSTANT DIFFUSION

If $\mathbf{D}$ does not depend on the variables $x^1, \ldots, x^M$ the first term in Eq. (2.4) vanishes. The remaining term has different properties whether $M = 2$ or $M \geqslant 3$. This is related to the fact that in the exponential representation

$$\mathbf{O} = \exp\mathbf{A}, \tag{3.1}$$

the antisymmetric matrices $\mathbf{A}(\mathbf{x}, t)$ all commute if $M = 2$, but not if $M \geqslant 3$. In fact, for $M = 2$, $\mathbf{A}$ can be written as

$$\mathbf{A} = \phi\boldsymbol{\sigma} \quad \text{with } \boldsymbol{\sigma} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{3.2}$$

and with a scalar $\phi(\mathbf{x}, t)$. Using (3.1) and (3.2) one simply obtains

$$\mathbf{O}^T\partial_\mu\mathbf{O} = (\partial_\mu\phi)\boldsymbol{\sigma} \tag{3.3}$$

and thus with (2.4)

$$2a^\nu = (\sqrt{\mathbf{D}}\boldsymbol{\sigma}\sqrt{\mathbf{D}})^{\mu\nu}\partial_\mu\phi.$$

By the antisymmetry and constancy of $\sqrt{\mathbf{D}}\boldsymbol{\sigma}\sqrt{\mathbf{D}}$ it follows that

$$\partial_\nu a^\nu = \operatorname{div}\ \mathbf{a} \equiv 0. \tag{3.4}$$

No similar condition holds if $M \geqslant 3$. Furthermore, Eq. (3.4) is the only restriction imposed on a^ν if $M = 2$. Both statements can be proved by showing that for an aribtrary field $\bar{a}^\nu$—sourcefree if $M = 2$—the equation

$$2\bar{a}^\nu = (\sqrt{\mathbf{D}}\,\bar{\mathbf{O}}^T(\partial_\mu\bar{\mathbf{O}})\sqrt{\mathbf{D}})^{\mu\nu}$$

can be solved for the orthogonal matrix field $\bar{\mathbf{O}}(\mathbf{x}, t)$. For this proof we may assume $\mathbf{D} \equiv \mathbb{1}$, which can be established by a linear change of variables (possibly depending on $x^{M+1}, \ldots, x^N$), thus

$$2\bar{a}^\nu = (\bar{O}^T\partial_\mu\bar{O})^{\mu\nu}. \tag{3.5}$$

The case $M = 2$ is trivial: here $\bar{\mathbf{O}}$ must have the form $\bar{\mathbf{O}} = \exp\bar{\phi}\boldsymbol{\sigma}$, and the equations for $\bar{\phi}$:

$$\partial_1\bar{\phi} = \bar{a}^2, \quad \partial_2\bar{\phi} = -\bar{a}^1$$

are integrable because of (3.4).

For $M \geqslant 3$ one can specify $\bar{\mathbf{O}}$ in an arbitrary hyperplane, $x^1 = \text{const} = x_0^1$ say, and integrate Eq. (3.5) along x^1 for at least a finite distance. The details of this procedure are shown in the Appendix.

4. DIFFUSION DEPENDING ON THE STATE OF THE SYSTEM

The results of Sec. 3 can be extended to $\mathbf{x}$-dependent still regular) diffusion matrices by use of tensor analysis, with the metric tensor chosen to be $D^{\mu\nu}(\mathbf{x}, t)$. For this the transformation properties of the LE under nonlinear changes of the variables $x^1, \ldots, x^M$ are essential. The standard perturbations $W_i(t)$ are assumed to remain unchanged,[6,7] and the same may hold for $x^{M+1}, \ldots, x^N$. From Eq. (1.1) it is clear that both $\dot{x}^\nu$ and f^ν are components of contravariant vectors, and therefore, by (1.2), also the b_i^ν with respect to the upper index. $D^{\mu\nu}$ is thus a twice contravariant tensor. The NID a^ν does not transform vectorlike,[6,7] but with the covariant derivative

$$b^\nu_{i;\lambda} = \partial_\lambda b_i^\nu + \Gamma^\nu_{\lambda\mu} b_i^\mu$$

it can be decomposed as

$$2a^\nu = b_j^\mu b^\nu_{j;\mu} - \Gamma^\nu_{\mu\lambda} D^{\mu\lambda}, \tag{4.1}$$

where the first term is now a vector. When $D^{\mu\nu}$ is chosen as the contravariant metric, the nontensor part of (4.1) is determined by $\mathbf{D}$ alone and it reads[7,8]

$$\Gamma^\nu_{\mu\lambda} D^{\mu\lambda} \triangleq \Gamma^\nu = -\theta^{-1}\partial_\mu(\theta D^{\mu\nu}), \tag{4.2}$$

$$\theta \triangleq (\det\mathbf{D})^{-1/2}. \tag{4.3}$$

Since $D^{\mu\nu}{}_{;\lambda} \equiv 0$ the vector part of (4.1) is

$$h^\nu \triangleq b_j^\mu b^\nu_{j;\mu} = -b^\mu_{j;\mu} b_j^\nu = -\theta^{-1}\partial_\mu(\theta b_j^\mu) b_j^\nu. \tag{4.4}$$

Thus

$$2a^\nu = h^\nu - \Gamma^\nu, \tag{4.5}$$

with the right-hand side given by (4.2)–(4.4).

It is interesting to note that a *given* NID can always be removed globally by a change of variables. This becomes clear from the transformation law of Γ^ν:[8]

$$\bar{\Gamma}^\nu = \Gamma^\mu\partial_\mu\bar{x}^\nu - D^{\lambda\mu}\partial_\lambda\partial_\mu\bar{x}^\nu.$$

The requirement

$$2\bar{a}^\nu = \bar{h}^\nu - \bar{\Gamma}^\nu = (h^\mu - \Gamma^\mu)\partial_\mu\bar{x}^\nu + D^{\lambda\mu}\partial_\lambda\partial_\mu\bar{x}^\nu \equiv 0 \tag{4.6}$$

can always be satisfied by some $\bar{\mathbf{x}}(\mathbf{x})$. (With $h^\mu = 0$ the new variables would be harmonic.[7,8])

We now consider the case $M = 2$ and seek for the generalization of condition (3.4) for $\mathbf{x}$-dependent diffusion. For this we evaluate the covariant divergence of the vector part h^ν. This can conveniently be done in locally Euclidian coordinates for which

$$\mathbf{D} = \mathbf{1}, \quad \partial_\nu\mathbf{D} = 0, \quad \text{and} \quad \Gamma^\nu_{\lambda\mu} = 0$$

at the considered point. Taking Eq. (2.4) in these variables and combining with Eq. (4.5) we obtain

$$\partial_\nu h^\nu = \partial_\nu\Gamma^\nu + \partial_\nu\partial_\mu(\sqrt{\mathbf{D}})^{\mu\nu} + \partial_\nu(\mathbf{O}^T\partial_\mu\mathbf{O})^{\mu\nu}.$$

Since $M = 2$ the last term vanishes for the same reason as in Sec. 3. The divergence of h^ν is therefore determined by $\mathbf{D}$ alone. The only tensor that can be constructed from the metric tensor and its first and second derivatives, and is linear in the second derivatives, is the curvature tensor .[8] Only

one scalar can be obtained from it in two dimensions, namely the curvature scalar R.[8] Hence the covariant divergence of h^{ν} must be R up to a numerical factor. A straightforward calculation yields

$$h^{\nu}_{;\nu} = \theta^{-1}\partial_{\nu}(\theta h^{\nu}) = R/2. \tag{4.7}$$

Expressions for R are given in Ref. 8 and in other standard textbooks. Equation (4.7) together with (4.5) and (4.2) generalizes the condition (3.4).

The $\mathbf{x}$ dependence of $\mathbf{D}$ does not induce any additional restrictions on the NID, at least not within a simply connected regularity domain of $\mathbf{D}$. Instead of working out the proof of this statement here, we will present it in the more general context of Part II.

5. SUMMARY AND DISCUSSION

Possible intrinsic connections between the drift and the diffusion coefficients of a FPE have been investigated, more precisely: the condition imposed on the noise-induced ("spurious") drift NID by a given diffusion matrix $\mathbf{D}$. It has been assumed that $\mathbf{D}$ is regular and that its dimension is equal to the number of independent noise sources M. (These assumptions will be dropped in Part II.)

The result differs whether $M = 1$, $M = 2$ or $M \geqslant 3$. While for $M = 1$ the NID is uniquely determined by $\mathbf{D}$, it is independent of $\mathbf{D}$ if $M \geqslant 3$. The case $M = 2$ is intermediate: the NID can be written as $a^{\nu} = (h^{\nu} - \Gamma^{\nu})/2$, where

$$\Gamma^{\nu} = -(\det \mathbf{D})^{1/2}\partial_{\mu}(D^{\mu\nu}/(\det \mathbf{D})^{1/2})$$

is determined by $\mathbf{D}$, and where h^{ν} can be any vector field satisfying

$$(\det \mathbf{D})^{1/2}\partial_{\nu}(h^{\nu}/(\det \mathbf{D})^{1/2}) = R/2,$$

R being the curvature scalar, when $\mathbf{D}$ is chosen to be the contravariant metric tensor. For constant diffusion this condition reduces to

$$\partial_{\nu}a^{\nu} = \operatorname{div}\mathbf{a} = 0 \quad (M = 2).$$

The result for $M \geqslant 3$ has an interesting consequence for Langevin equations in the Stratonovich sense: to a given LE

$$\dot{x}^{\nu} = f^{\nu}(\mathbf{x}, t) + b_i^{\nu}(\mathbf{x}, t)\xi_i \quad (\nu = 1, ..., M)$$

there always exists a stochastically equivalent LE

$$\dot{x}^{\nu} = \tilde{f}^{\nu}(\mathbf{x}, t) + \tilde{b}_i^{\nu}(\mathbf{x}, t)\xi_i$$

with an arbitrary $\tilde{f}^{\nu}$ (e.g. $\tilde{f}^{\nu} \equiv 0$), since any NID can be generated by some $\tilde{b}_i^{\nu}$ obeying $\tilde{b}_i^{\mu}\tilde{b}_i^{\nu} = D^{\mu\nu} = b_i^{\mu}b_i^{\nu}$. In other words: when the noise influence is specified by the diffusion (or covariance) matrix alone, the lack of information is equivalent to the whole deterministic part of the LE.

An additional result states that any *given* NID can be forced to zero globally by an appropriate change of the state variables (leaving the noise sources unaltered). This holds for $M \geqslant 1$.

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APPENDIX

We show that for $M \geqslant 3$ Eq. (3.5)

$$(\mathbf{O}^T\partial_{\mu}\mathbf{O})_{\mu\nu} = -a_{\nu} \quad (\nu = 1, ..., M) \tag{A1}$$

can be solved for $\mathbf{O}$ with any given nonsingular field a_{ν}. (In this context neither the prefactor of a_{ν} nor the distinction between upper and lower indices are important. Furthermore we will replace the symbol ∂_{μ} by $_{,\mu}$.) For this we specify $\mathbf{O}$ in a hyperplane $x^1 = \text{const} = x_0^1$ and then integrate with respect to x^1. The derivative $\mathbf{O}_{,1}$ can always be written as

$$\mathbf{O}_{,1} = \mathbf{OA} \tag{A2}$$

with an antisymmetric $\mathbf{A}$, since the antisymmetric matrices are the generators of the rotation group. The solution of (A2) is then

$$\mathbf{O}(x^1, \cdot) = \mathbf{O}(x_0^1, \cdot)T\exp\int_{x_0^1}^{x^1}\mathbf{A}(\xi, \cdot)\,d\xi, \tag{A3}$$

T being the ordering operator with respect to x^1. We thus have to derive $\mathbf{A}$ from (A1) and to make sure that it remains antisymmetric during the integration.

Rewriting (A1) as

$$a_{\nu} = (\mathbf{O}^T{}_{,\mu}\mathbf{O})_{\mu\nu} = (\mathbf{O}^T\mathbf{O}_{,\mu})_{\nu\mu} \tag{A4}$$

and inserting (A2) gives

$$A_{\nu 1} = a_{\nu} - (\mathbf{O}^T\mathbf{O}_{,\alpha})_{\nu\alpha} \quad (\alpha \geqslant 2). \tag{A5}$$

For $\nu \geqslant 2$ this specifies the elements $A_{\nu 1} = -A_{1\nu}$ by the values of $\mathbf{O}$ in a hyperplane $x^1 = \text{const}$. Antisymmetry imposes

$$A_{11} = 0 = a_1 - (\mathbf{O}^T\mathbf{O}_{,\alpha})_{1\alpha} \quad (\alpha \geqslant 2). \tag{A6}$$

This condition can be met in the initial hyperplane since, with the antisymmetric $\mathbf{B}$ defined by $\mathbf{O}_{,2} = \mathbf{OB}$, Eq. (A6) only requires

$$B_{12} = a_1 - (\mathbf{O}^T\mathbf{O}_{,\gamma})_{1\gamma} \quad (\gamma \geqslant 3), \tag{A7}$$

which means that $\mathbf{O}$ can be specified arbitrarily in the directions $x^3, ..., x^M$. The persistence of (A6) for $x^1 \neq x_0^1$ is less trivial. By taking the derivative of Eq. (A6) with respect to x^1 one obtains

$$a_{1,1} = (-\mathbf{AO}^T\mathbf{O}_{,\alpha} + \mathbf{O}^T\mathbf{O}_{,\alpha}\mathbf{A} + \mathbf{A}_{,\alpha})_{1\alpha}. \tag{A8}$$

Since by (A5)

$$A_{1\alpha,\alpha} = -a_{\alpha,\alpha} + (\mathbf{O}^T\mathbf{O}_{,\beta})_{\alpha\beta,\alpha} \quad (\alpha, \beta \geqslant 2),$$

Eq. (A8) is equivalent to

$$\begin{aligned} a_{\nu,\nu} &= \operatorname{div}\mathbf{a} \\ &= (\mathbf{O}^T\mathbf{O}_{,\alpha}\mathbf{A} - \mathbf{AO}^T\mathbf{O}_{,\alpha})_{1\alpha} \\ &\quad + (\mathbf{O}^T{}_{,\alpha}\mathbf{O}_{,\beta} + \mathbf{O}^T\mathbf{O}_{,\alpha\beta})_{\alpha\beta} \quad (\alpha, \beta \geqslant 2). \end{aligned} \tag{A9}$$

From this it can easily be rederived that $\mathbf{a}$ must be source-free if $M = 2$. For the case of interest, $M \geqslant 3$, we note that $(\mathbf{O}^T\mathbf{O}_{,\alpha}\mathbf{A})_{1\alpha}$ involves elements of $\mathbf{A}$ which have not yet been determined. Thus Eq. (A9) is another condition for $\mathbf{A}$, and for $M = 3$ $\mathbf{A}$ is now completely specified. For $M \geqslant 4$ the solution of (A1) is not uniquely determined by initial conditions on a hyperplane.

A problem may arise if

$$(\mathbf{O}^T\mathbf{O}_{,\alpha})_{1\beta} \quad (\alpha, \beta \geqslant 2) \tag{A10}$$

is symmetric in α, β. In that case the additional elements of $\mathbf{A}$

are eliminated from (A9) (the trace of the product of a symmetric and an antisymmetric matrix vanishes), and the integrating procedure stops, because Eq. (A9) cannot in general hold any more. We note however that the integration can always be performed along a finite interval of x^1, since in the initial hyperplane the expression (A10) can be chosen arbitrarily far from being symmetric. This also means that the value x_c^1 where the solution fails to exist is not determined by a alone (consider different initial conditions on a hyperplane close to x_c^1) but by the initial conditions as well.

To summarize: starting from an arbitrary hyperplane in x-space a solution of (A1) can be constructed at least within a hyperslab of finite thickness.

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Properties of the noise-induced ("spurious") drift. II. Simplifications of Langevin equations

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In a previous paper (I) we studied the interrelations between the coefficients of Fokker–Planck equations associated to a restricted class of Langevin equations. We now discuss the general case of an arbitrary state-dependent diffusion matrix **D**, which, in particular, may be singular. Moreover the number of noise sources, M, is now allowed to exceed the rank L of **D** and even the number N of state variables. The noise-induced drift **a** is always found to split into a part which is determined by **D** alone and a contribution which must lie within the tangential subspace $\mathcal{T}_{\|}$ spanned by the noise coefficients ($\mathcal{T}_{\|}$ is specified by **D**). This second contribution strongly depends on L: While for $L = 1$ it vanishes, it is unrestricted (within $\mathcal{T}_{\|}$) for $L \geqslant 3$. If $L = 2$, a simple characterization is only found under the assumptions of I; the condition on the divergence derived therein is now proved to be sufficient. Langevin equations can often be simplified in two respects: The number of noise sources is always reducible to L (unless $L = 2$) without change of any terms in the Fokker–Planck equation, and if either $L = 1$ or a set of conditions holds, new variables can be introduced in such a way that only L of them are directly affected by noise. (Both reductions together lead to the form considered in I.) For $L \geqslant 3$ any given Langevin equation can be replaced by a stochastically equivalent one, the deterministic part of which has an arbitrarily chosen component in $\mathcal{T}_{\|}$.

1. INTRODUCTION

The purpose of this paper is to generalize and complete results that we have presented in Ref. 1 (hereafter referred to as I) concerning the "spurious" or "noise-induced" drift. This drift arises in the study of stochastic processes that can be described by Langevin equations (LE)[2–5]

$$\dot{x}^{\nu} = f^{\nu}(\mathbf{x}, t) + b_i^{\nu}(\mathbf{x}, t)\xi_i(t). \tag{1.1}$$

Following the notations of I we understand a summation over double indices. The state of the system is characterized by the variables $x^{\nu}(\nu = 1, ..., N)$, which are driven by the random forces $\xi_i(i = 1, ..., M)$. We assume these forces to be white standard-Gaussian noise and interpret (1.1) in the Stratonovich sense.[1–4,6]

Equivalently, such a process can be described by the Fokker–Planck equation (FPE) for the probability density of **x**

$$\partial_t p(\mathbf{x}, t) = -\partial_{\nu} F^{\nu}(\mathbf{x}, t)p(\mathbf{x}, t) + \tfrac{1}{2}\partial_{\nu}\partial_{\mu} D^{\nu\mu}(\mathbf{x}, t)p(\mathbf{x}, t). \tag{1.2}$$

The diffusion matrix $D^{\nu\mu}$ is related to the noise coefficients b_i^{ν} by

$$D^{\nu\mu} = b_i^{\nu} b_i^{\mu}, \tag{1.3}$$

whereas the drift

$$F^{\nu} = f^{\nu} + a^{\nu}, \tag{1.4}$$

contains the noise-induced drift (NID)

$$a^{\nu} = \tfrac{1}{2} b_i^{\mu} \partial_{\mu} b_i^{\nu}, \tag{1.5}$$

besides the "deterministic" drift **f**.

As in I our main topic will be to find the conditions on the NID once the diffusion matrix **D** is specified. We then also know the restrictions on the deterministic drift $\bar{\mathbf{f}}$ of any process being stochastically equivalent to the given one (i.e., having the same FPE). They are surprisingly weak.

Here we consider the general case of a possibly singular, state-dependent diffusion matrix. The rank L of **D**, the number N of variables, and the number M of noise sources may all be different. We therefore have to discuss also the possibility of reducing the number of noise sources to a minimal one (namely L).

In some cases it is even possible to introduce new variables in such a way that only the first L of them couple to the noise explicitly. Then the diffusion matrix is regular within this subspace of the configuration space, the case already discussed in I. We establish the necessary and sufficient conditions for this.

2. POSSIBLE FORMS OF THE LANGEVIN EQUATION

We now assume the diffusion matrix $D^{\nu\mu}$ to be given and look for the possible forms of the noise coefficients b_i^{ν}. If the rank L of **D** is less than the dimension N of the configuration space, **D** splits the local tangential space $\mathcal{T}(\mathbf{x})$ into a L-dimensional part $\mathcal{T}_{\|}$ invariant under **D**

$$\mathbf{D}\mathcal{T}_{\|} = \mathcal{T}_{\|}, \tag{2.1}$$

and an $(N - L)$-dimensional part orthogonal to **D**

$$\mathbf{D}\mathcal{T}_{\perp} = 0. \tag{2.2}$$

According to the decomposition [cf. (1.3)]

$$D^{\mu\nu} = b_I^{\mu} b_I^{\nu}, \tag{2.3}$$

(we now use capital indices running from 1 to M and reserve small ones for 1 to L) the noise coefficients $\mathbf{b}_I$, as vectors in $\mathcal{T}$, have to span $\mathcal{T}_{\|}$. Their minimal number is therefore given by L. One particular decomposition uses the normalized eigenvectors $\mathbf{u}_{(i)}$ of **D**

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$$b_i^\nu = \sqrt{D_{(i)}}\, u_{(i)}^\nu,$$

where

$$D^{\mu\nu} u_{(i)}^\nu = D_{(i)} u_{(i)}^\mu, \quad u_{(i)}^\nu u_{(j)}^\nu = \delta_{ij}. \tag{2.4}$$

Obviously, this choice is not invariant under transformations of the variables.

Any other decomposition $\bar{b}_i^\nu$ must be related linearly to b_i^ν

$$\bar{b}_i^\nu = O_{ij} b_j^\nu, \tag{2.5}$$

by an orthogonal matrix **O**, as follows from (2.3),

$$O_{ki} O_{kj} = \delta_{ij}, \tag{2.6}$$

or, in the case of a decomposition with more than L noise sources

$$\bar{b}_I^\nu = O_{Ij} b_j^\nu, \tag{2.7}$$

by a rectangular $M \times L$ matrix O fulfilling

$$O_{Ki} O_{Kj} = \delta_{ij}. \tag{2.8}$$

For a given FPE we therefore can construct LE's with L or more fluctuating forces. The deterministic drift **f** of the LE is then related to the drift **F** of the FPE by Eqs. (1.4) and (1.5).

3. REDUCTION OF THE NUMBER OF NOISE SOURCES

The question arises whether it is possible to reduce the number of noise sources for a given LE to the minimal number $L = \text{rank } \mathbf{D}$ without affecting the drift **f**. For given noise coefficients $B_I^\nu (I = 1, ..., M > L)$ we look for new ones b_i^ν $(i = 1, ..., L)$ with the same NID [cf. Eq. (1.5)]

$$\tfrac{1}{2} b_i^\mu \partial_\mu b_i^\nu = \tfrac{1}{2} B_I^\mu \partial_\mu B_I^\nu, \tag{3.1}$$

and the same diffusion matrix

$$b_i^\nu b_i^\mu = B_I^\nu B_I^\mu. \tag{3.2}$$

As we know from Eq. (2.5) the new coefficients are determined by Eq. (3.2) up to an orthogonal matrix

$$b_i^\nu = O_{ij} \beta_j^\nu, \tag{3.3}$$

where β_j^ν is some (minimal) decomposition of **D**. Equation (3.1) now reads as an equation for **O** [using (3.2)]

$$\beta_j^\mu (\partial_\mu O_{kj}) O_{ki} \beta_i^\nu = (\partial_\mu B_I^\mu) B_I^\nu - (\partial_\mu \beta_i^\mu) \beta_i^\nu, \tag{3.4}$$

with given right-hand side lying in $\mathcal{T}_\parallel$.

For $L \geqslant 3$ we will show in Sec. 5 that this equation is solvable for arbitrary right-hand side lying in $\mathcal{T}_\parallel$, at least in some finite region about an arbitrarily chosen point of the configuration space.

For $L = 1$ the left-hand side vanishes identically since the only orthogonal matrix is the identity. On the other hand B_I must be linearly related to the single vector $\boldsymbol{\beta}$ [cf. Eq. (2.7)]

$$B_I^\nu = \bar{O}_I \beta^\nu, \quad \bar{O}_I \bar{O}_I = 1, \tag{3.5}$$

by an $M \times 1$ matrix $\bar{\mathbf{O}}$. Therefore the right-hand side of Eq. (3.4) vanishes too

$$\beta^\nu \bar{O}_I \partial_\mu (\bar{O}_I \beta^\mu) - \beta^\nu \partial_\mu \beta^\mu = \beta^\nu \bar{O}_I (\partial_\mu \bar{O}_I) \beta^\mu$$
$$= \tfrac{1}{2} \beta^\nu (\partial_\mu \bar{O}_1 \bar{O}_1) \beta^\mu = 0.$$

Thus the noise coefficients can be reduced to a single-column matrix.

For $L = 2$ no generally valid result could be derived. (If we allow the deterministic drift **f** to change, it is of course trivial to find a stochastically equivalent LE with just L noise sources even for $L = 2$.)

4. REDUCTION OF THE NUMBER OF FLUCTUATING VARIABLES

In view of the possibility to reduce the number of noise sources to L (unless $L = 2$) it is tempting to ask whether one can also introduce new variables $\bar{\mathbf{x}}$ instead of **x** such that only the first L of them couple directly to the noise sources. Geometrically this means that the tangential subspace $\mathcal{T}_\parallel$ can be interpreted as the tangential space of a subspace $\bar{x}^{L+1}(\mathbf{x})$, ..., $\bar{x}^N(\mathbf{x}) = \text{const}$ of the configuration space.

The noise coefficients transform according to (cf. I)

$$\bar{b}_i^\nu = \frac{\partial \bar{x}^\nu}{\partial x^\mu} b_i^\mu, \tag{4.1}$$

and we are looking for a transformation with

$$\bar{b}_i^\nu = 0 \quad \forall \nu > L. \tag{4.2}$$

This is possible iff there exist coefficients C_{ij}^k such that

$$b_i^\mu \partial_\mu b_j^\nu - b_j^\mu \partial_\mu b_i^\nu = C_{ij}^k b_k^\nu, \tag{4.3}$$

i. e., the left-hand side lies within $\mathcal{T}_\parallel$. For $M = 1$ this is trivially fulfilled because of the antisymmetry in i and j.

Proof: Let $\mathcal{T}_\perp$ be spanned by γ^a, $a = L + 1, ..., N$, i.e.,

$$\gamma_\mu^a b_i^\mu = 0. \tag{4.4}$$

Equation (4.2) is then equivalent to

$$\bar{\gamma}_\nu^a \equiv \gamma_\mu^a \frac{\partial x^\mu}{\partial \bar{x}^\nu} = 0 \quad \forall \nu \leqslant L. \tag{4.5}$$

This is a Pfaffian system

$$\omega^a \equiv \gamma_\mu^a \, dx^\mu = 0, \tag{4.6}$$

which according to the Frobenius–Cartan Theorem[7] is completely integrable iff

$$d\omega^a \wedge \omega^{L+1} \wedge \cdots \wedge \omega^N = 0 \quad \forall a > L, \tag{4.7}$$

or, equivalently, iff there exist coefficients $A_{b\nu}^a$ such that

$$\partial_\nu \gamma_\mu^a - \partial_\mu \gamma_\nu^a = A_{b\nu}^a \gamma_\mu^b - A_{b\mu}^a \gamma_\nu^b. \tag{4.8}$$

Multiplying by $b_i^\mu b_j^\nu$ and using the orthogonality (4.4) one easily derives (4.3), Q. E. D.

Of course, the condition (4.3) depends only on $\mathcal{T}_\parallel$ and not on the particular noise coefficients spanning $\mathcal{T}_\parallel$.

5. PROPERTIES OF THE NID

We now investigate the intrinsic properties of the NID, i.e., the set of NID's compatible with a given diffusion matrix. In view of Sec. 3 we may assume that exactly L noise sources are involved (the case $L = 2$ will be treated separately).

Starting from an arbitrarily chosen decomposition $D^{\mu\nu} = \beta_j^\mu \beta_j^\nu$ of the diffusion matrix we obtain all possible noise coefficients by orthogonal transformations

$$b_i^\nu = O_{ij}\beta_j^\nu. \tag{5.1}$$

The NID is then given by

$$2a^\nu = b_i^\mu b_{i,\mu}^\nu = \beta_i^\mu \beta_{i,\mu}^\nu + \beta_i^\mu O_{ki} O_{kj,\mu}\beta_j^\nu. \tag{5.2}$$

(We have introduced the shorthand notation $A_{,\nu}$ for $\partial_\nu A$.) This formula is closely analogous to Eq. (2.4) of I. In what follows we focus on the O-dependent term, which we denote by $-k^\nu$,

$$k^\nu = \beta_i^\mu O_{ki,\mu} O_{kj}\beta_j^\nu, \tag{5.3}$$

where the orthogonality of O has been used. Note that all NID's belonging to the same $\mathbf{D}$ differ by $\mathbf{k}/2$ and consequently also the deterministic drifts $\mathbf{f}$, $\bar{\mathbf{f}}$ of stochastically equivalent LE's, since

$$f^\nu + a^\nu = F^\nu = \bar{f}^\nu + \bar{a}^\nu \quad \text{and} \quad a^\nu - \bar{a}^\nu = k^\nu/2. \tag{5.4}$$

In I the special case $\beta_i^\nu \equiv \delta_i^\nu$ ($\nu = 1,...,M = L$) has been discussed with the result that in three or more dimensions $\mathbf{k}$ is unrestricted, in two dimensions its divergence must vanish, and in one dimension it has to vanish identically. We will show that analogous results hold in the more general case, namely;

(i) k^ν must lie in the local subspace $\mathcal{T}_\parallel$ spanned by the noise coefficients or by $\mathbf{D}$, respectively.

(ii) For $L = 1$, $\mathbf{k}$ has to vanish identically.

(iii) For $L = 2$, a simple result only holds if $N = M = 2$, as well. Then we find $(k^\nu(\det \mathbf{D})^{-1/2})_{,\nu} = 0$, or, in the covariant notation of I, $k^\nu_{;\nu} = 0$ [equivalent to $h^\nu_{;\nu} = R/2$, Eq. (4.7) of I].

(iv) For $L \geqslant 3$, $\mathbf{k}$ can be chosen arbitrarily within $\mathcal{T}_\parallel$ at least in a finite region about an arbitrarily chosen point $\mathbf{x}$ of the configuration space, i.e., up to global restrictions.

Proof:

(i) From (5.3) we take immediately

$$k^\nu = K_i\beta_i^\nu, \tag{5.5}$$

with some coefficients K_i. We have now to investigate the restrictions on $\mathbf{k}$, by considering

$$K_i = O_{ki} O_{kj,\mu}\beta_j^\mu, \tag{5.6}$$

as an equation for $\mathbf{O}$, whereby the existence of solutions will possibly imply some conditions on K_i. It is sufficient to look for solutions $\mathbf{O}$ being connected with the identity $\mathbf{1}$, since a new solution is found by multiplication with a constant matrix $\mathbf{O}$.

(ii) For $L = 1$ the only orthogonal matrix is the identity itself, yielding vanishing $\mathbf{K}$.

(iii) The two-dimensional orthogonal matrices are generated by the only antisymetric matrix $\boldsymbol{\sigma}$:

$$\mathbf{O}(\mathbf{x}) = e^{\phi(\mathbf{x})\boldsymbol{\sigma}},$$

with

$$\boldsymbol{\sigma} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \phi(\mathbf{x}) = \text{scalar function}. \tag{5.7}$$

Therefore Eq. (5.3) takes the form

$$k^\nu = \phi_{,\mu}(\beta_1^\nu \beta_2^\mu - \beta_2^\nu \beta_1^\mu). \tag{5.8}$$

The term in parenthesis is antisymmetric in μ, ν and has the only nonvanishing component

$$\beta_1^1\beta_2^2 - \beta_2^1\beta_1^2 \equiv \det\boldsymbol{\beta} \equiv (\det \mathbf{D})^{1/2}. \tag{5.9}$$

The resulting equations for ϕ

$$\begin{aligned} \phi_{,1} &= k^2(\det \mathbf{D})^{-1/2}, \\ \phi_{,2} &= -k^1(\det \mathbf{D})^{-1/2}, \end{aligned} \tag{5.10}$$

are solvable iff

$$(k^\nu(\det \mathbf{D})^{-1/2})_{,\nu} = 0, \tag{5.11}$$

as stated.

(iv) for $L \geqslant 3$ the proof essentially parallels the one given in the Appendix of I. We note that an arbitrary path $\mathbf{x}(\tau)$ in configuration space corresponds to a path $\mathbf{O}(\mathbf{x}(\tau))$ in the orthogonal group $\mathbf{SO}(L)$, along which $\mathbf{O}$ changes by the action of a generator $\mathbf{A}(\tau)$:

$$d\mathbf{O}/d\tau = \mathbf{O}(\tau)\mathbf{A}(\tau), \tag{5.12}$$

with the solution

$$\mathbf{O}(\tau) = \mathbf{O}(\tau_0) T \exp \int_{\tau_0}^{\tau} d\tau' \, \mathbf{A}(\tau'), \tag{5.13}$$

T being the ordering operator with respect to τ. The generators of $\mathbf{SO}(L)$ are the antisymmetric matrices $\mathbf{A}$.

We construct a solution of (5.3) or, equivalently, (5.6) by specifying $\mathbf{O}$ on a hyperplane and integrating along paths perpendicular to it according to (5.13). Since $\mathcal{T}_\parallel$ is at least three-dimensional ($L \geqslant 3$) we can assume that it contains just the x^1 and x^2 direction, possibly after a change of coordinates, and at least within a finite region around an arbitrarily chosen point $\mathbf{x}_{(0)}$,

$$\beta_1^1 \neq 0, \quad \delta \equiv \begin{vmatrix} \beta_1^1 & \beta_2^1 \\ \beta_1^2 & \beta_2^2 \end{vmatrix} \neq 0. \tag{5.14}$$

We then choose the hyperplanes

$$\mathcal{H}(\tau) = \{\mathbf{x} | x^1 = x^1_{(0)} + \tau\}, \tag{5.15}$$

and the paths

$$\mathbf{x}(\tau) = \mathbf{x}(0) + (\tau, 0, ..., 0), \quad \mathbf{x}(0) \in \mathcal{H}(0), \tag{5.16}$$

starting at $\mathcal{H}(0)$. Equation (5.12) then reads in components

$$O_{ij,1} = O_{ik}A_{kj}, \tag{5.17}$$

where $\mathbf{A}$ must be chosen such that (5.6) holds

$$K_i = A_{ij}\beta_j^1 + O_{ki}O_{kj,\alpha}\beta_j^\alpha \quad \alpha = 2, ..., N. \tag{5.18}$$

For $i \neq 1$ it can be solved for $A_{a1} = -A_{1a}$ ($a, b = 2, ..., L$)

$$A_{a1} = (K_a - O_{ka}O_{kj,\alpha}\beta_j^\alpha - A_{ab}\beta_b^1)/\beta_1^1, \tag{5.19}$$

leaving $A_{ab} = -A_{ba}$ undetermined. Due to the antisymmetry of $\mathbf{A}$ the remaining equation represents a condition to be fulfilled *within* each hyperplane $\mathcal{H}(\tau)$

$$K_i\beta_i^1 = \beta_i^1 O_{ki}O_{kj,\alpha}\beta_j^\alpha. \tag{5.20}$$

In the initial hyperplane $\mathcal{H}(0)$ we can construct $\mathbf{O}$ analogously by integrating along the x^2 direction with an antisymmetric matrix $\mathbf{B}$. The single equation (5.20)

$$\beta_i^1 B_{ij}\beta_j^2 = K_i\beta_i^1 - \beta_i^1 O_{ki}O_{kj,\rho}\beta_j^\rho, \tag{5.21}$$

($\rho = 3, ..., N$) now fixes only one component of $\mathbf{B}$ and is always solvable, since $\delta \neq 0$. A particularly simple soution is

$$\mathbf{O}(x^1_{(0)}, x^2, ..., x^N) = \begin{pmatrix} \cos\psi & -\sin\psi & & \\ \sin\psi & \cos\psi & & \mathbf{0} \\ & & \mathbf{0} & \mathbf{1} \end{pmatrix}, \tag{5.22}$$

with

$$\psi(x^1_{(0)}, x^2, ..., x^N) = \psi(x^1_{(0)}, x^2_{(0)}, x_3, ..., x_N) + \int_{x^2_{(0)}}^{x^2} dx^2\, K_i \beta^1_i/\delta, \tag{5.23}$$

and arbitrarily chosen angle ψ in the subhyperplane $x^1 = x^1_{(0)}, x^2 = x^2_{(0)}$. To ensure Eq. (5.20) in each hyperplane $\mathscr{H}(\tau)$ we must investigate its derivative along the τ direction

$$(K_i \beta^1_i)_{,1} = (\beta^1_i O_{ki} O_{kj,\alpha} \beta^\alpha_j)_{,1}, \tag{5.24}$$

which can be brought into the form

$$M_{ab} A_{ab} = F(\mathbf{K}, \boldsymbol{\beta}, \mathbf{O}, \mathbf{O}_{,\alpha}, \mathbf{O}_{,\alpha\beta}). \quad (a, b, \alpha, \beta \geqslant 2). \tag{5.25}$$

The right-hand side is completely determined within $\mathscr{H}(\tau)$, whereas the left-hand side contains the yet undetermined part A_{ab} of A, which can be chosen to solve (5.25) as long as the antisymmetric part of the matrix

$$M_{ab} = (\beta^\alpha_a \beta^1_b O_{i1} + \beta^\alpha_b \beta^1_1 O_{ia} + \beta^\alpha_1 \beta^1_a O_{ib})(O_{ij} \beta^1_j)_{,\alpha} \tag{5.26}$$

does not vanish. It is easy to verify that the explicit solution (5.23) fulfills this condition at least in a finite part of $\mathscr{H}(0)$ if the initial angle is chosen suitably. Therefore it remains valid for a finite interval $\tau > 0$, i.e., we have constructed a solution of (5.3) within a finite region around an arbitrarily chosen point, Q. E. D. The size of this region certainly depends on the choice of the undetermined parts of **A** and **B**. Unfortunately, we are not able to prove it to be extendable throughout the whole configuration space by an appropriate choice of those parts.

6. CONCLUSIONS

The description of stochastic processes by Langevin equations involves the noise sources explicitly, in contrast to the Fokker–Planck description which only deals with the stochastic properties of the variables. Usually one is interested in these last properties and identifies stochastically equivalent processes.

As a remnant of the explicit coupling to the noise sources the noise-induced (or spurious) drift enters the drift part of the Fokker–Planck equation. In this paper (and its first part[1]) we investigated the interrelation between the NID and the diffusion matrix **D**. The NID can always be split into a contribution determined by **D** alone and a second part lying within the invariant tangential subspace $\mathscr{T}_\parallel$ of **D** (spanned by the noise coefficients). This second part depends qualitatively on the rank L of **D**: While for $L = 1$ it vanishes, it is unrestricted (within $\mathscr{T}_\parallel$) for $L \geqslant 3$. The case $L = 2$ is more involved and depends on the dimension of the configuration space and the number of noise sources, as well.

With this result we also find that each given Langevin equation has a stochastically equivalent counterpart, the "deterministic" drift of which has an arbitrarily chosen component in $\mathscr{T}_\parallel$ (if $L \geqslant 3$). Further simplifications of Langevin equations were investigated: While the number of noise sources can always be reduced to L ($L \neq 2$) without affecting the noise-induced drift and the remaining terms of the Fokker–Planck equation, it is not in general possible to introduce new variables in such a way that only L of them are directly perturbed (unless $L = 1$). The conditions for such a reduction were formulated.

It should be noted that some of the main results were only proved within some finite regions around arbitary points in **x** space. The existence of global restrictions is thus not excluded.

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A concept of spin 1/2 approximation in the quantum theory of lattice Bose systems

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We give a model independent description of criteria under which expectation values of observables associated with a finite part of the lattice Bose system can be made to converge to those of the associated Fermi or finite spin system.

1. MOTIVATION

In the series of papers Refs. 1–3 we have investigated the question of a possible "metamorphosis" of bosons into fermions from a mathematical point of view, by looking for fermion field algebras inside bicommutants of given Bose field algebras. In Refs. 4–8 we have considered a few physical cases in which the bosonlike properties of finite spin or Fermi systems arise in local observations, see also Ref. 9. It suggested that we state the problem of (almost) Fermi or spin states of the given Bose systems and further that we look for constraints which must be imposed on Bose systems to make them exhibit the Fermi-like properties.

Our idea is based on looking for the "metamorphosis" prescriptions which allow the expectation values of observables associated with a finite part of the Bose system to converge to those of the associated Fermi or finite spin system. Then locally bosons can be used as approximations of fermions or conversely. In this connection the basic observation of Refs. 7 and 8 was that the spin-$\frac{1}{2}$ approximation of the initially given Bose system should arise as a result of the "metamorphosis": Each Bose degree of freedom must be then replaced by the spin-$\frac{1}{2}$ degree.

From a physical point of view, the spin-$\frac{1}{2}$ approximation becomes of interest for these Bose systems, whose low-lying (the vicinity of the ground state energy) excitations play the dominating role: It is, for example, known that the system ϕ^4 in one, and two space–time dimensions can be made to exhibit the Fermi-like properties, and that its Fermi (i.e., spin-$\frac{1}{2}$) limit can be introduced; it is a respective one or two space–time dimensional Ising model.[9–17] Our aim is to give the model independent criteria under which the spin-$\frac{1}{2}$ approximation works for an arbitrary Bose system on the lattice.

In Sec. 2 we construct a one-parameter family of (in general non-Fock) lattice Bose systems, whose irreducibility sectors (IDPS($|f,\lambda\rangle$)) are labelled by a respective family of generating vectors $\{|f,\lambda\rangle\}_{\lambda\in[0,\infty)}$. Theorem 1 and 2 prove that each IDPS($|f,\lambda\rangle$) can be embedded into a larger space so that a one-parameter family of coupled pairs (Bose system-thermal reservoir) arises for each separately chosen and fixed (for all λ) equilibrium temperature value $\beta = 1/kT$. Then $\langle f,\lambda | a_s^* a_s | f,\lambda\rangle$ equals the statistical Bose distribution, which in the limit $\lambda\to\infty$ goes over to the statistical Fermi distribution. It allows us to interpret each $\{|f,\lambda\rangle\}_{\lambda\in[0,\infty)}$ system to give an account of the one-parameter family of couplings of the lattice boson to the gas of its quanta, subject to the $_\beta\langle f,\lambda | a_s^* a_s | f,\lambda\rangle_\beta = 1/\{\exp[\beta\omega_B^s(\lambda,\beta)]-1\}$ constraint for all $\lambda\in[0,\infty)$ and a singly chosen fixed value of $\beta>0$.

With each β we have associated its own β th family $\{\omega_s^B(\lambda,\beta)\}$ of frequencies of the quantum gas. In Sec. 3, we investigate the limiting properties of the expectation values [in between the elements of IDPS($|f,\lambda\rangle$)] of the normal ordered bounded operator functions $:F_J(a^*,a):$ associated with the J th finite part $\{a_s^*,a_s\}_{s\in J}$ of the Bose system, as $\lambda\to\infty$.

Theorems 6 and 7 establish here the Fermi limits for all possible $:F_J(a^*,a):$ including in this number operators of local time translations $\exp(itH_B^J)$.

An essential feature of this quantum picture is that the quantum system needs to be in contact with the temperature nonzero thermostat. Then the temperature dependent domain for quantum operators is introduced, so that if the energy separation between the energy levels is large enough, or if the gap between the lowest two and the others is large enough, we find that the two-level (spin-$\frac{1}{2}$) approximation of the quantum system allows a satisfactory reproduction of its basic properties, like, e.g., the structure of the set of transition probabilities, or expectation values of bounded operators.

2. FIELD-RESERVOIR INTERACTION ON THE LINEAR BOSE LATTICE: ALMOST FERMI, BOSE DISTRIBUTIONS IN QUANTUM THEORY

Let us consider a countable sequence of the identical elementary quantum systems, each one described in terms of a separable Hilbert space $h_s = h$, $s = 0, \pm 1, \pm 2,\ldots$ enumerating single systems (sites of a linear lattice). Let $f_s\in h_s$, we introduce a notion of a product vector $f = \Pi_{s=-\infty}^{+\infty}\otimes f_s \in \Pi_s\otimes h_s$, $\|f\| = \Pi_s\|f_s\| < \infty$ and of the incomplete direct product space IDPS(f) $= \Pi_s^f\otimes h_s$ generated by the product vector f.[18] The reducible representation of the CCR algebra in $\Pi_s\otimes h_s$ is assumed to be generated by a sequence $\{a_s^*, a_s; [a_s, a_{s'}^*]_-\subset\delta_{ss'}\mathbf{1}_\beta, [a_s,a_{s'}]_- = 0 = [a_s^*, a_{s'}^*]_-\}$ such that a unique (up- to unitarity) state $|0\rangle$, $a_s|0\rangle = 0$ $\forall s$ exists in $\Pi_s\otimes h_s$. Its irreducible component recieved by the restriction to a particular IDPS(f), we denote $\{a_s^*,a_s,f\}_{s=0,\pm1,\ldots}$. Let $\{a_s^*,a_s,f\}_{s=0,\pm1,\ldots}$ be associated with some self-interacting lattice Bose system, whose dynamics is governed by the Hamiltonian of the form $H = \Sigma_s\{H_s^0 + \Sigma_{t\neq s}W_{st}^{\rm int}\}$, provided the finite volume restriction and suitable boundary conditions are imposed. Both H_s^0 and $W_{st}^{\rm int}$ can be completely expressed in terms of a_s^*, a_s; for an example of the ϕ_2^4:

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$$H = H_B = V \sum_{s=-N}^{+N} \left\{ \frac{p_s^2}{2} + \frac{m^2+2}{2} x_s^2 + \gamma x_s^4 - x_s x_{s+1} \right\},$$
$$[p_s, x_r]_- = -i\delta_{sr}, \quad m,\gamma > 0. \tag{2.1}$$

We make now a simplifying assumption and consider H in its single-site approximation by $H^0 = \Sigma_s H_s^0$. For a while let us restrict considerations to a single site of the lattice. Let A be an observable associated with a single elementary quantum system whose total Hamiltonian is denoted by $\mathscr{H}$. We look (possibly in h) for the state vector $|0(\beta)\rangle$ with the property:

$$\langle A \rangle_\beta = (0(\beta)|A|0(\beta)) = Z^{-1}(\beta) \sum_n (n|A|n)\exp(-\beta E_n),$$
$$\mathscr{H}|n) = E_n|n), \quad (n|m) = \delta_{nm},$$
$$\sum_n |n)(n| = \mathbb{1}_B, Z(\beta) = \mathrm{Tr}\exp(-\beta\mathscr{H}), \tag{2.2}$$

so that $|0(\beta)\rangle$ becomes a temperature dependent state if $\beta = 1/kT$. However we have in this connection the following no-go observation.

Lemma 1: There is no state $|0(\beta)\rangle$ in h.

Proof: Indeed, if we expand $|0(\beta)\rangle$ in the energy basis (a nondegenerate discrete spectrum for $\mathscr{H}$ is assumed), $|0(\beta)\rangle = \Sigma_n |n) f_n(\beta)$, then the following identity immediately follows,[18–21]

$$\bar{f}_n(\beta) f_m(\beta) = Z^{-1}(\beta)\exp(-\beta E_n)\delta_{nm}, \tag{2.3}$$

which cannot be reconciled with the c-number properties of the functions f_n, f_m.

To circumvent this difficulty, we shall use a trick of Refs. 19–21 and introduce a subsidiary tilde system, playing the role of the reservoir:

$$\tilde{\mathscr{H}}|\tilde{n}) = E_n|\tilde{n}), \quad (\tilde{n}\,|\,\tilde{m}) = \delta_{nm}, \quad \sum_n |\tilde{n})(\tilde{n}| = \tilde{\mathbb{1}}_B,$$
$$|n,\tilde{n}) \in h \otimes \tilde{h}, \quad (\tilde{n},n'|A|m,\tilde{m}') = (n'|A|m)\delta_{nm'},$$
$$f_n(\beta) := |\tilde{n})\exp(-\beta E_n/2)\cdot Z^{-1/2}(\beta),$$
$$|0(\beta)) = Z^{-1/2}(\beta) \sum_n |n,\tilde{n})\exp(-\beta E_n/2). \tag{2.4}$$

For an elementary spin $\frac{1}{2}$ it implies

$$\mathscr{H} = \omega b^* b, \quad [b,b^*]_+ = \mathbb{1}_F,$$
$$|0(\beta))_F = \{1/[1+\exp(-\beta\omega)]^{1/2}\}\{|0) + \exp(-\beta\omega/2)\cdot b^*\tilde{b}^*|0)\} = \exp(-iG)|0), \tag{2.5}$$
$$|0) = e_0 \otimes \tilde{e}_0 = |0,\tilde{0}), \quad G = -i\Theta(\beta)\{\tilde{b}b - b^*\tilde{b}^*\},$$
$$\cosh\Theta(\beta) = [1+\exp(-\beta\omega)]^{-1/2}$$

(h becomes a two-dimensional space), so that:

$${}_F(0(\beta)|b^* b|0(\beta))_F = \exp(-\beta\omega)/[1+\exp(-\beta\omega)] \tag{2.6}$$

follows. For a boson system (elementary Schrödinger one)

$$\mathscr{H} = \omega a^* a, \quad [a,a^*]_- \subset \mathbb{1}_B,$$
$$|0(\beta))_B = [1-\exp(-\beta\omega)]^{1/2} \times \exp[a^*\tilde{a}^*\exp(-\beta\omega/2)]|0) = \exp(-iG)|0), \tag{2.7}$$

$$G = -i\Theta(\beta)(\tilde{a}a - a^*\tilde{a}^*),$$
$$\cosh\Theta(\beta) = [1-\exp(-\beta\omega)]^{-1/2},$$

we get

$${}_B(0(\beta)|a^* a|0(\beta))_B = \exp(-\beta\omega)/[1-\exp(-\beta\omega)]. \tag{2.8}$$

Assume now that the experimental limitations impose a lower (say positive) bound $\omega_0 \leqslant \omega_s$ on the observable frequency spectrum and let $\beta \gg 0$ (low temperature limit). Then

$${}_B(0(\beta)|a^* a|0(\beta))_B \simeq \exp(-\beta\omega) \simeq {}_F(0(\beta)|b^* b|0(\beta))_F \tag{2.9}$$

and thus the temperatures increase restores, up to a significant level, a difference between the Bose and Fermi distributions in the above. Our aim in this place is to construct the mechanism, which is capable of compensating the difference between the Fermi and Bose distributions so that both cases become indistinguishable within experimental accuracy limits, at nonzero finite temperatures. Define now a mapping U_λ in h according to:

$$U_\lambda f = f_\lambda \in h, \quad |k) = e_k,$$
$$(e_k, e_l) = \delta_{kl}, \quad \sum_k \tilde{e}_k \otimes e_k = \mathbb{1}_B,$$
$$U_\lambda e_k = e_k^\lambda = \left(\frac{1}{1+\lambda}\right)^{\Sigma_j^k\,{}_1(j-1)/2} \cdot e_k,$$
$$f = \sum_k f_k e_k, \quad k = 0,1,\cdots, \quad \lambda \in [0,\infty), \tag{2.10}$$

so that $\|e_k^\lambda\| = [1/(1+\lambda)]^{\Sigma_j^k\,{}_1(j-1)}$ for all $k > 1$, $\|e_0^\lambda\| = \|e_0\|$, $\|e_1^\lambda\| = \|e_1\|$. Assume further to have fixed a countable sequence $\{f_s\}_{s=0,\pm1,\cdots}$ of state vectors in h, and define

$$|f) = \prod_s \otimes (f \otimes \tilde{e})_s,$$
$$\prod_s (h \otimes \tilde{h})_s \ni |f,\lambda) = \prod_s \otimes (f^\lambda \otimes \tilde{e}_0)_s,$$
$$f_s^\lambda = U_\lambda f_s / \|U_\lambda f_s\|,$$
$$\|U_\lambda f_s\|^2 = \sum_k |f_s^k|^2 [1/(1+\lambda)]^{\Sigma_j^k\,{}_1(j-1)}. \tag{2.11}$$

Then the following holds true:

Theorem 1: Assume the product vector $|f,\lambda)$ in $\Pi_s \otimes (h \otimes \tilde{h})_s$ to be constructed so that: $f_s^0 \in \mathbb{R}$, $f_s^0 > 0$, $\forall s$, $|f,\lambda) = \Pi_s \otimes (f^\lambda \otimes \tilde{e}_0)_s$,

$$\sum_s \ln\left[\frac{\|f_s\|}{f_s^0}\left(1 + \sum_{k=1}^\infty \frac{k|f_s^k|^2}{\|f_s\|^2}\right)^{1/2}\right] < \infty. \tag{2.12}$$

Then for each fixed value of $\lambda \in [0,\infty)$ there exists in IDPS($|f,\lambda)$) an associated vector $|\Theta,\lambda)$ satisfying

$$(\Theta,\lambda\,|a_s^* a_s\,|\Theta,\lambda) = \sinh^2\Theta_s(\lambda) = (f,\lambda\,|a_s^* a_s\,|f,\lambda). \tag{2.13}$$

Proof: In the basis $\{e_k\}_{k=0,1,\cdots}$ of h we have

$$h = h_s \ni f_s^\lambda = \sum_{k=0}^\infty f_s^k e_s^\lambda (1/\|U_\lambda f_s\|), \tag{2.14}$$

so that for all s the formula

$$(f,\lambda\,|a_s^* a_s\,|f,\lambda)$$

$$= \sum_{u=1}^{\infty} \frac{k\,|f_s^k|^2}{\|U_\lambda f_s\|^2}\left(\frac{1}{1+\lambda}\right)^{\Sigma_j^k{}_{,(j-1)}} \tag{2.15}$$

can be used to define a sequence $\{\Theta_s = \Theta_s(\lambda)\}_{s=0,\pm 1,\ldots}$ by demanding

$$(f,\lambda\,|a_s^* a_s\,|f,\lambda): = \sinh^2\Theta_s(\lambda). \tag{2.16}$$

Any choice of the set $\{\Theta_s(\lambda)\}_{s=0,\pm 1,\ldots}$ subject to the above identity determines a state $|\Theta,\lambda\rangle$ in $\Pi_s \otimes (h \otimes \tilde{h})_s$ and, because $|f,\lambda\rangle$ is a state in the same space [i.e., $\Pi_s \otimes (h \otimes \tilde{h})_s$] the sufficient condition to allow $|\Theta,\lambda\rangle$ and $|f,\lambda\rangle$ to belong to the same IDPS = IDPS($|f,\lambda\rangle$) is $(f,\lambda\,|\Theta,\lambda) \neq 0$.[18]

This last condition holds true, if for all fixed $\lambda \in [0,\infty)$ there is

$$\prod_s \frac{1}{\cosh\Theta_s(\lambda)} \frac{f_s^0}{\|U_\lambda f_s\|} = \exp\left[-\sum_s \ln\left(\frac{\|U_\lambda f_s\|}{f_s^0}\cosh\Theta_s(\lambda)\right)\right] \neq 0, \tag{2.17}$$

which needs

$$\sum_s \ln\left\{\frac{\|U_\lambda f_s\|}{f_s^0} \times\left[1+\sum_k |f_s^k|^2 \frac{k}{\|U_\lambda f_s\|^2}\left(\frac{1}{1+\lambda}\right)^{\Sigma_j^k{}_{,(j-1)}}\right]^{1/2}\right\} < \infty. \tag{2.18}$$

Notice that each argument under the sign of ln exceeds the value 1 for all λ, and so by taking $\lambda > 0$ we have improved a convergence of the series. Hence if the inequality of Theorem 1 holds true, we have guaranteed the fulfillment of the last inequality for all λ.

Theorem 2: Under notations of Theorem 1, let us introduce $\Omega_s^B(\lambda) = \ln[\coth^2\Theta_s(\lambda)]$ and $\Omega_s^F = 2\ln(|f_s^0/f_s^1|)$ provided $f_s^1 \neq 0$. Then for all s the quantity

$$n_s^B(\lambda) = (\Theta,\lambda\,|a_s^* a_s\,|\Theta,\lambda) \tag{2.19}$$

converges to

$$n_s^F = 1/(1+\exp\Omega_s^F) \tag{2.20}$$

as $\lambda \to \infty$.

Proof: Because of

$$\Omega_s(\lambda) = \ln\frac{1+\sinh^2\Theta_s(\lambda)}{\sinh^2\Theta_s(\lambda)}$$

we have $\sinh^2\Theta_s(\lambda) = 1/[\exp\Omega_s(\lambda) - 1]$. But by virtue of (2.15) the limit

$$\lim_{\lambda\to\infty}\Omega_s(\lambda) = \ln\frac{2|f_s^1|^2 + |f_s^0|^2}{|f_s^1|^2} \tag{2.21}$$

immediately follows, so that indeed

$$\lim_{\lambda\to\infty} 1/[\exp\Omega_s(\lambda) - 1] = 1/(1 + |f_s^0|^2/|f_s^1|^2) = 1/(1+\exp\Omega_s^F), \tag{2.22}$$

which proves the theorem.

Now, notice that $\Omega_s^B(\lambda)$, Ω_s^F arise as dimensionless quantities, thus providing us with a continuous spectrum of dimensional frequencies for each fixed value of $\beta\omega_s(\lambda,\beta) = \Omega_s(\lambda) \in \mathbb{R}^+$. Here, we may demand $\beta = 1/kT$ to be a common fixed factor, characterizing a thermal equilibrium of any (possibly finite) fraction J of lattice sites. Then by fixing β we have associated with each sth site, $s \in J$, a frequency curve $\omega_s(\lambda,\beta)$ for which an immediate identity,

$$\omega_s(\lambda,\beta) = \ln\left(\frac{1+n_s^B(\lambda)}{n_s^B(\lambda)}\right)^{1/\beta}, \tag{2.23}$$

follows from the definition of Ω_s^B. In the dimensional description, the "enforcing" of the spin $\frac{1}{2}$ approximation of the given Bose system, can be understood as the transition through a λ family of frequencies $\{\omega_s(\lambda,\beta)\}_{s\in J}$ at a fixed thermal equilibrium. Since for $\lambda \gg 1$, $n_s^B(\lambda)$ can be made not to differ significantly from n_s^F, the notion of an almost-Fermi, Bose distribution seems to be suitable for $n_s^B(\lambda)$ in that case.

3. SPIN-$\frac{1}{2}$ APPROXIMATION ON THE BOSE LATTICE

We consider a fixed finite subset $J \ni s$ of elementary quantum systems (sites) in our infinite assembly, subject to a particular field-reservoir interaction of Theorems 1 and 2.

We are interested now in investigating effects of the λ constraint of the previous section on the finite part of the system only. Let us extract from $|f,\lambda\rangle$ a finite tensor product part $|f,\lambda\rangle_J = \Pi_{s\in J} \otimes f_s^\lambda$ and define a vector $|\lambda\rangle$, associated with $|f,\lambda\rangle_J$ by putting

$$(\lambda\,|a_s^* a_s\,|\lambda) = \sinh^2\Theta_s(\lambda)\cdot\prod_{s\in J}\|U_\lambda f_s\|^2. \tag{3.1}$$

Notice that such a step is impossible in the infinite J limit. Here

$$|\lambda) = \prod_{s\in J} \otimes\, U_\lambda f_s = \left\{\prod_{s\in J} U_\lambda^s\right\}\prod_{s\in J}\otimes f_s := U_\lambda|0), \tag{3.2}$$

$$|0) = \lim_{\lambda\to 0}|\lambda),$$

and the redundant $\tilde{e}_0 \otimes \cdots \otimes \tilde{e}_0$ terms in the tensor product were for simplicity omitted. Analogously, with $|\Theta,\lambda\rangle_J$ in hand, we get

$$(\vartheta\,|a_s^* a_s\,|\vartheta) = \prod_{s\in J}\|U_\lambda f_s\|^2\,{}_J(\Theta,\lambda\,|a_s^* a_s\,|\Theta,\lambda\rangle_J. \tag{3.3}$$

Let us add in this place the following:

Lemma 2: Denote P_E, a spectral projection on the subspace h_E of h consisting of states whose energy is bounded by E. For all finite values of E the map U_λ is invertible in h_E. Moreover there exists the map

$$U_{\lambda\lambda'}: f_{\lambda'} \to f_\lambda, \quad U_{\lambda\lambda'} = U_{\lambda\lambda'}^{-1} \neq U_{\lambda'\lambda}^*. \tag{3.4}$$

Proof: By restricting to h_E we guarantee that for $f \in h_E$ the vectors $U_\lambda^{-1} f$ will also belong to h_E. Here

$$U_\lambda^{-1} e_k = e_\lambda^k = (1+\lambda)^{\Sigma_j^k{}_{,(j-1)/2}}\cdot e_k. \tag{3.5}$$

Obviously in h_E, $f_\lambda = U_\lambda f = U_\lambda U_{\lambda'}^{-1} U_{\lambda'} f = U_{\lambda\lambda'} f_{\lambda'}$ and $U_{\lambda\lambda'}^{-1} f_\lambda = U_{\lambda'} U_\lambda^{-1} U_\lambda f = f_{\lambda'}$. Consequently $(\lambda\,|a_s^* a_s\,|\lambda)$ $= (0|U_\lambda^* a_s^* a_s U_\lambda|0)$, where $|0) = \lim_{\lambda\to 0}|\lambda)$.

The existence of U_λ^{-1} allows us to generate λ "motions" by the use of operations $U_{\lambda\lambda'}$. Therefore, we should in

where

$$|d) = \lim_{\lambda\to\infty} |d,\lambda), \quad :F_J(\sigma^+,\sigma^-): = :F_J(a^*\to\sigma^+,a\to\sigma^-):.$$

Proof: Immediate by arguments of Theorem 5, if we notice that $\lim_{\lambda\to\infty} |d,\lambda) = \mathbb{1}_F^J|d) = |d)$, $:F_J(\sigma^+,\sigma^-):$ we call a Fermi limit of $:F_J(a^*,a):$.

Suppose, we have given an IDPS-generating vector $|f,\lambda)$. Let $H_B^J(\lambda)$ be a normal ordered with respect to $\{a_s^*, a_s\}_{s\in J}$ polynomial (or a bounded function) generator of the time translations for the lattice Bose system $\{a_s^*,a_s,|f,\lambda)\}$, $\lim_{\lambda\to\infty} H_B^J(\lambda) = \underset{\sim}{H}_B^J$, $\lim_{\lambda\to 0} H_B^J(\lambda) = H_B^J$. By denoting $H_B^J(\lambda,a^*,a) = H_B^J(\lambda)$ we indicate a (possible) λ-dependence of the expansion coefficients of the generator H_B^J associated with IDPS($|f,\lambda)$).

Theorem 7: Suppose $\mathbb{1}_F^J$ to be a projection on some spectral subspace of $\lim_{\lambda\to\infty} H_B^J(\lambda) = \underset{\sim}{H}_B^J$. Then

$$\lim_{\lambda\to\infty} (d,\lambda)\exp[iH_B^J(\lambda)t]|d,\lambda) = (d|\exp(iH_F^J t)|d) \tag{3.15}$$

for all $|d,\lambda)\in d_\lambda^J$ and $H_F^J = \underset{\sim}{H}_B^J$ $(a^*\to\sigma^+, a\to\sigma^-)$.

Proof: We have

$$\lim_{\lambda\to\infty} (d,\lambda|\exp[iH_B^J(\lambda)t]|d,\lambda) = (d|\mathbb{1}_F^J\exp(i\underset{\sim}{H}_B^J t)\mathbb{1}_F^J|d) = \sum_n \frac{(it)^n}{n!}(d|\mathbb{1}_F^J(\underset{\sim}{H}_B^J)^n\mathbb{1}_F^J|d), \tag{3.16}$$

where $(d|\mathbb{1}_F^J\underset{\sim}{H}_B^J\mathbb{1}_F^J|d)$ identifies the only part $H_F^J = H_B^J(a^*\to\sigma^+, a\to\sigma^-)$ of

$$\underset{\sim}{H}_F^J + (\mathbb{1}_B^J - \mathbb{1}_F^J)\underset{\sim}{H}_B^J\mathbb{1}_F^J + \mathbb{1}_F^J\underset{\sim}{H}_B^J(\mathbb{1}_B^J - \mathbb{1}_F^J) + (\mathbb{1}_B^J - \mathbb{1}_F^J)\underset{\sim}{H}_B^J(\mathbb{1}_B^J - \mathbb{1}_F^J),$$

which while acting in d_λ^J will never produce any vector from beyond this domain. We easily find that $(d|\mathbb{1}_B^J\underset{\sim}{H}_B^J\mathbb{1}_F^J|d) = (d|H_F^J|d)$, and analogously for all n, because

$$\underset{\sim}{H}_B^J = H_F^J + (\mathbb{1}_B^J - \mathbb{1}_F^J)\underset{\sim}{H}_B^J(\mathbb{1}_B^J - \mathbb{1}_F^J). \tag{3.17}$$

COMMENTS

1. For a particular example of ϕ_1^4 the λ dependence can be understood as the combined mass-coupling constant parametrization of the model. Just in the large mass -strong coupling regime, the Schwinger functions of ϕ_1^4 were shown to tend to suitably normalized Schwinger functions of the one-dimensional Ising model.[10-17] In this case the Ising limit of ϕ_1^4 arises via letting all higher energy levels of the (involved) anharmonic oscillator to become arbitrarily large if compared with the lowest two: The gap between these last can be kept insensitive to the limiting procedure. Obviously an assumption that ϕ_1^4 lives in the thermal bath is crucial in this point.

For ϕ_2^4 the λ dependence must give account of the (relative) weakening of the inbetween -sites couplings if compared with the single site contribution to the total energy. For weakly coupled chains the spin approximation (and spin $\frac{1}{2}$ in this number) arguments become reliable at nonzero finite temperatures; see, e.g., Ref. 15. For higher dimensions the "critical point" ($\lambda = \infty$ for ϕ_1^4) presumably corresponds to a true transition point for the system.

2. Quite similar (to ϕ_1^4) arguments were applied in Ref. 8 to get a deformation of the quantum pendulum into an elementary spin $\frac{1}{2}$. The basic goal was there a construction of the quantum analog of the classically arising angular momentum of plane pendulum (its average is nonzero for rotating motions). It concerns the still not finally resolved question of the relation classical-quantum for spin and Fermi systems; see, e.g., Ref. 1–8, but especially Ref. 22.

3. Though going a bit beyond the scope of the present paper, let us discuss shortly a fundamental question of the roots of the famous sine-Gordon –Thirring model equivalence[23-27]: spin-$\frac{1}{2}$ particles are here believed to arise in the original Bose theory. In fact, as shown in Ref. 26, the two-dimensional Coulomb gas of the charge $\pm q$ particles, at the inverse temperature β is equivalent to the sine-Gordon system with the Coleman's coupling constant given by $\beta_c = (4\pi\beta)^{1/2}q$. Then for $\beta q^2 \geqslant 2$ the dipole phase of the Coulomb system arises, while in the interval $0 \leqslant \beta q^2 < 2$ the system lives in the charged plasma phase. The value $\beta q^2 = 2$ corresponds to $\beta_c^2 = 8\pi$ which is the instability point in the Coleman's study of the sine-Gordon vacuum.[25-27]

Just below the critical threshold $\beta q^2 = 2$ the plasma phase of the Coulomb system (and of the equivalent to it, sine-Gordon system) can be rigorously described in terms of the Thirring model, while above $\beta q^2 = 2$ the dipole gas occurs (the ultraviolet divergences cause some people to refer to the "nonexistence" of the sine-Gordon model).

Notice that formally, we can investigate this phase transition at a fixed temperature $1/\beta$, by varying the charge value q only. Then a one-parameter family of the sine-Gordon systems arises and an analogy with consideration of the previous sections appears to be striking: Recall that Coleman conjectured in Ref. 25 that spectra of the sine-Gordon and Thirring model Hamiltonians do coincide in the interval indicated above. For further investigations on this subject and the spin $\frac{1}{2}$ xyz linear chain approximation of the sine-Gordon system, see, e.g., Ref. 28.

4. In connection with Lemma 2, it seems reasonable to give an explanation for when the finite energy bound E is of no matter (at least approximately). Namely let E be a fixed single site energy bound, $h_E = P_E h$. With $H = \Sigma_n E_n e_n \otimes \bar{e}_n$ (nondegenerate discrete spectrum) in mind, we denote $2s = n_E = \{\max n, (n|H|n) \leqslant E, |n) = e_n\}$. The triple $\mathbf{S}_E = P_E \mathbf{S} P_E$ with $\mathbf{S}$ given by the Holstein–Primakoff formula,[5]

$$S^+ = \sqrt{2s}\,a^*(1 - a^*a/2s)^{1/2},$$

$$S^- = \sqrt{2s}\,(1 - a^*a/2s)^{1/2}a, \quad S^3 = s - a^*a$$

defines an irreducible in h_E representation of the SU(2) Lie algebra corresponding to spin $s = n_E/2$. Here the following relations are immediate:

$$[S^+,S^-]_- = 2S^3, \quad [S^3,S^\pm]_- = \pm S^\pm,$$

and h naturally splits into the two orthogonal subspaces h_E, $(1 - P_E)h$ respectively, which are invariant under the action

principle restrict all f_s in the above to belong to h_E.

Theorem 3: Let $\mathbb{1}_F$ be a projection on the linear span of $\{e_0,e_1\}$ in h. U_λ converges to $\mathbb{1}_F$ as $\lambda\to\infty$.

Proof: Observe that $\mathbb{1}_F = :\exp(-a^*a): + a^*:\exp(-a^*a):a$ so that $\mathbb{1}_F$ projects on $\lim_{\lambda\to\infty} f_s^\lambda = \Sigma_{k=0,1} f_s^k e_k = f_s^\infty$. Consequently

$$\lim_{\lambda\to\infty} |\lambda) = \mathbb{1}_F|0) = \mathbb{1}_F|\lambda) \quad \forall\ \lambda\in[0,\infty). \tag{3.6}$$

Corollary: $U_\lambda^J = \Pi_{s\in J}\otimes U_\lambda^s$ converges to $\Pi_{s\in J}\otimes \mathbb{1}_F^s = \mathbb{1}_F^J$ in $\Pi_{s\in J}\otimes h_s$ as $\lambda\to\infty$.

Proof: Through an immediate calculation one can check that

$$\left(\prod_{s\in J}\otimes\ \mathbb{1}_F^s\right)\prod_{s\in J}\otimes f_s = \prod_{s\in J}\otimes f_s^\infty = \mathbb{1}_F^J\prod_{s\in J}\otimes f_s^\lambda = \mathbb{1}_F^J\prod_{s\in J}\otimes f_s\,. \tag{3.7}$$

Now take into account the $(n+m)$-fold totally antisymmetric tensor $f_{r_1\cdots r_n s_1\cdots s_m}$ and denote $\epsilon_{r_1\cdots r_n}$, the n-fold Levi–Civita tensor. We define

$$f^c_{r_1\cdots r_n s_1\cdots s_m} = f_{r_1\cdots r_n s_1\cdots s_m}\cdot\epsilon_{r_1\cdots r_n}\cdot\epsilon_{s_1\cdots s_m}\,. \tag{3.8}$$

Assume now to have defined in $\Pi_{s\in J}\otimes h_s$ the bounded functions of Bose generators $\{a_s^*,a_s\}_{s\in J}$ which are of the form

$$:F^c(a^*,a): = \sum_{nm}(f^c_{nm},a^{*n}a^m) = \sum_{nm}\sum_{\{r\}\in J}\sum_{\{s\}\in J} f^c_{r_1\cdots r_n s_1\cdots s_m}\times a^*_{r_1}\cdots a^*_{r_n}a_{s_1}\cdots a_{s_m}. \tag{3.9}$$

Theorem 4: Let us denote by $\mathscr{U}_B^J$ a representation of the CCR algebra generated in $\Pi_{s\in J}\otimes h_s$ by $\{a_s^*,a_s\}_{s\in J}$. In the bicommutant $(\mathscr{U}_B^J)''$ of $\mathscr{U}_B^J$ there arises a representation of the CAR algebra associated with the cyclic vector of the former, so that the following identity holds true:

$$\lim_{\lambda\to\infty}(\lambda|:F^c(a^*,a):|\lambda) = (0|:F(b^*,b):|0) = (\lambda|:F(b^*,b):|\lambda) \quad \forall\lambda\in[0,\infty). \tag{3.10}$$

Here $:F(b^*,b): = \Sigma_{nm}(f_{nm},b^{*n}b^m)$ and on $\mathbb{1}_F^J\Pi_{s\in J}\otimes h_s$ it holds that $[b(f),b(g)^*]_- = (f,\bar g)\mathbb{1}_F^J$.

Proof: Notice that in $\Pi_{s\in J}\otimes h_s$ we have satisfied

$$\mathbb{1}_F^J = \prod_{s\in J}\otimes\ \mathbb{1}_F^s = \sum_n\frac{1}{n!}\sum_{\{r\}\in J} a^*_{r_1}\cdots a^*_{r_n}: \times\exp\left(-\sum_{s\in J}a_s^*a_s\right):a_{r_1}\cdots a_{r_n}\cdot\epsilon_{r_1\cdots r_n}\,. \tag{3.11}$$

It is the operator unit of the CAR algebra arising in $(\mathscr{U}_B^J)''$ by virtue of Refs. 1–3. By Theorem 3 we have

$$\lim_{\lambda\to\infty}(\lambda|:F^c(a^*,a):|\lambda) = (0|\mathbb{1}_F^J:F^c(a^*,a):\mathbb{1}_F^J|0), \tag{3.12}$$

but by virtue of projection theorems of Ref. 3, we find that $\mathbb{1}_F^J:F^c(a^*,a):\mathbb{1}_F^J$ is just equivalent to $:F(b^*,b):$ on all vectors taken from $\mathbb{1}_F^J\Pi_{s\in J}\otimes h_s$ (it is a Fock space for the representation).

In the above construction a concept of the spin-$\frac{1}{2}$ approximation explicitly appears due to the following theorem.

Theorem 5: Suppose, we have constructed in IDPS($|f,\lambda)$) a domain $\mathscr{D}_\lambda^J$ received by applying all possible polynomials $W_J(a^*,a)$ of variables $\{a_s^*,a_s\}_{s\in J}$ on the generating vector $|f,\lambda)$. Furthermore let: $F_J(a^*,a)$: be a bounded function of $\{a_s^*,a_s\}_{s\in J}$. For each vector $|\mathscr{D},\lambda)\in\mathscr{D}_\lambda^J$ there holds

$$\lim_{\lambda\to\infty}(\mathscr{D},\lambda|:F_J(a^*,a):|\mathscr{D},\lambda) = (f|\mathbb{1}_F^J W_J(a^*,a)^*:F_J(a^*,a):W_J(a^*,a)\mathbb{1}_F^J|f) = (f|\mathbb{1}_F^J:G_J(a^*,a):\mathbb{1}_F^J|f) = (f|:G_J(\sigma^+,\sigma^-):|f), \tag{3.13}$$

where

$$|f) = \lim_{\lambda\to\infty}|f,\lambda), \quad [\sigma_s^-,\sigma_t^+]_- = 0, \quad s\neq t, \quad [\sigma_s^-,\sigma_s^+]_+ = \mathbb{1}_F^s \quad \forall s\in J,$$

and

$$G_J(a^*,a): = W_J^*F_JW_J = \sum_{nm}\sum_{\{s\}}\sum_{\{t\}} G_{s_1\cdots s_n r_1\cdots r_m}a^*_{s_1}\cdots a^*_{s_n}a_{r_1}\cdots a_{r_m}$$

arises as a normal ordered expression for $W_J^*F_JW_J$ while $:G_J(\sigma^+,\sigma^-): = :G_J(a^*\to\sigma^+,a\to\sigma^-):$.

Proof: By Theorem 3 and Corollary, Theorem 5 immediately follows if neither of indices in the sequence $\{s\}$ or $\{t\}$ in the sum appears more than once. Then it is enough to notice that $\mathbb{1}_F^s a_s^*\mathbb{1}_F^s = \sigma_s^+$, $\mathbb{1}_F^s a_s\mathbb{1}_F^s = \sigma_s^-$ and $\mathbb{1}_F^s(a_s^*a_s)^k\mathbb{1}_F^s = (\sigma_s^+\sigma_s^-)^k$, $k\geqslant 1$.

If any index is repeated more than once (or at least once) in either $\{s\}$ or $\{t\}$, then the $\mathbb{1}_F^J(\cdots)\mathbb{1}_F^J$ "sandwiching" makes the corresponding term vanish. Consequently, due to $(\sigma_s^+)^2 = 0 = (\sigma_s^-)^2$ we can replace each $(a_s^*)^k$, $(a_t)^l$ by $(\sigma_s^+)^k$, $(\sigma_t^-)^l$, respectively.

Obviously Theorem 5 does not in any sense contradict Theorem 4. One knows that with a finite number ($J\ni s$) of spin-$\frac{1}{2}$'s in hand, an application of the Jordan–Wigner formulas,[5] allows us to rewrite $:G_J(\sigma^+,\sigma^-):$ in terms of pure Fermi variables $:G_J(\sigma^+,\sigma^-): = :G_J'^c(b^*,b):$, where by Theorem 4, $:G_J'^c(b^*,b):$ has its corresponding $:G_J'(a^*,a):$.

Assume now a single site energy bound of Lemma 2 to be infinite, so that all finite energy levels at each site are allowed. We apply to $|f,\lambda)$ the set of all polynomials $\{W_J(a_\lambda^*,a_\lambda)\}$ with respect to $\{a_{s\lambda}^* = U_\lambda^J a_s^*(U_\lambda^J)^{-1}, a_{s\lambda} = U_\lambda^J a_s(U_\lambda^J)^{-1}\}_{s\in J}$ and denote $\{W_J(a_\lambda^*,a_\lambda)|f,\lambda)\} = d_\lambda^J \subset$ IDPS($|f,\lambda)$). Notice that in d_λ^J we have $[a_{s\lambda},a_{t\lambda}^*]_- \subset \delta_{st}\mathbb{1}_B$. By making use of d_λ^J we are able to assign to each bounded function $:F_J(a^*,a):$ its "Fermi limit."

Theorem 6: For each bounded normal ordered operator function $:F_J(a^*,a):$ and all vectors $|d,\lambda)\in d_\lambda^J$ it holds that

$$\lim_{\lambda\to\infty}(d,\lambda|:F_J(a^*,a):|d,\lambda) = (d|:F_J(\sigma^+,\sigma^-):|d), \tag{3.14}$$

of S. Consequently the $P_E(\cdot)P_E$ sandwiching selects an irreducible component of the SU(2) based on h_E.

Let us now choose one more energy bound $\Delta \ll E$ and $h_\Delta = P_\Delta h$ with $n_\Delta \ll 2s$. In h_Δ the following holds:

$$\sqrt{2s}\, T_\Delta^+ = P_\Delta S_E^+ P_\Delta \simeq P_\Delta \sqrt{2s}\, a^* P_\Delta,$$

$$\sqrt{2s}\, T_\Delta^- = P_\Delta S_E^- P_\Delta \simeq P_\Delta \sqrt{2s}\, a^* P_\Delta,$$

where the triple $T^\pm, J_z$ with $J_z = S_E^3$ generates the E(2) group Lie algebra in h. It so happens that due to $n_\Delta \ll s$ the factors $(1 - n_\Delta/s)^{1/2} \simeq 1$ can be neglected when applying S on h. Furthermore: $[J_z, T^\pm]_- = \pm T^\pm$, $[T^+, T^-]_- = \mathbb{1}_B$ so that under the additional (to P_E) P_Δ sandwiching, there is no essential difference between SU(2), i.e., h_E and E(2), i.e., h, provided $n_\Delta \ll 2s$.

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Nonlinear internal symmetry

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A theory of n scalar fields is outlined in which the equations of motion are invariant under all nonsingular global transformations of the fields amongst themselves, whether linear or nonlinear.

It was recently shown to be possible to formulate a gauge theory of a noncompact internal symmetry group.[1,2] This formalism will be used in the present paper to construct a theory that posseses a high degree of nonlinear internal symmetry. A theory of n scalar fields $\phi_i(x)$ will be exhibited whose Lagrangian is invariant under all nonsingular transformations of the form

$$\phi'_i(x) = F_i[\phi_1(x), \phi_2(x),...,\phi_n(x)]. \tag{1}$$

These transformations may be arbitrarily nonlinear as long as they are one-to-one and continuously differentiable. Implementation of this symmetry excludes the possibility of an explicit mass term for the fields $\phi_i(x)$. A particular solution of the field equations will be presented.

The symmetry transformation (1) is global since the functions F_i do not depend explicitly upon the space-time point x. Therefore the derivatives of the fields ϕ_i transform linearly

$$\phi'_{i,\mu}(x) = J_{ij}(x)\phi_{j,\mu}(x) \tag{2}$$

where $J_{ij}(x)$ is the partial derivative of the function $F_i[\phi(x)]$ with respect to $\phi_j(x)$

$$J_{ij}(x) = \partial F_i[\phi(x)]/\partial\phi_j(x), \tag{3}$$

and the subscript comma mu means $\partial/\partial x^\mu$. The derivatives $\phi_{i,\mu}$ transform as a vector under the group GL(n, $\mathbb{C}$). In order to make objects that are invariant under this transformation, it is necessary to introduce a metric tensor $g_{ij}(x)$ that is Hermitian and positive and that transforms as

$$g_{ij}(x) = [J^{-1}(x)]^*_{\ ki} g_{kl}(x)[J^{-1}(x)]_{lj}\ . \tag{4}$$

In matrix notation, Eqs. (2) and (4) read

$$\phi'_{,\mu}(x) = J(x)\,\phi_{,\mu}(x) \tag{5}$$

and

$$g'(x) = J^{-1\dagger}(x)\,g(x)\,J^{-1}(x)\ . \tag{6}$$

Evidently the form

$$L(\phi) = \phi^\dagger_{,\mu}(x)\,g(x)\,\phi^{,\mu}(x) \tag{7}$$

is invariant.

A suitable covariant derivative of the metric tensor g may be defined as

$$g(x)_{;\mu} = g(x)_{,\mu} + g(x)\,A_\mu(x) + A^\dagger_\mu(x)\,g(x) \tag{8}$$

provided the $n\times n$ matrix of gauge fields A_μ transforms as

$$A'_\mu(x) = J(x)\,A_\mu(x)\,J^{-1}(x) + J(x)_{,\mu}J^{-1}(x)\,. \tag{9}$$

For then it follows from equations (6), (8), and (9) that $g_{;\mu}$ transforms like g

$$g(x)'_{;\mu} = J^{-1\dagger}(x)\,g(x)_{;\mu}J^{-1}(x)\,. \tag{10}$$

The curvature tensor is

$$F_{\mu\nu}(x) = A_\mu(x)_{,\nu} - A_\nu(x)_{,\mu} + [A_\mu(x), A_\nu(x)] \tag{11}$$

and transforms as

$$F'_{\mu\nu}(x) = J(x)\,F_{\mu\nu}(x)\,J^{-1}(x)\,. \tag{12}$$

The Lagrange density

$$L = \phi^\dagger_{,\mu}\,g\phi^{,\mu} + \tfrac{1}{4}m^2\mathrm{tr}(g_{;\mu}\,g^{-1}g^{;\mu}g^{-1}) - \tfrac{1}{2}e^{-2}\,\mathrm{tr}(F^\dagger_{\mu\nu}\,gF^{\mu\nu}\,g^{-1}) \tag{13}$$

is invariant under the nonlinear internal symmetry transformation defined by equations (1), (4), and (9). The number e is a dimensionless coupling constant and m is mass.

The covariant derivatives of $F^{\sigma\tau}$ and $g^{\ \nu}$ are

$$F^{\sigma\tau}_{\ ;\mu} = F^{\sigma\tau}_{\ ,\mu} + [F^{\sigma\tau}, A_\mu] \tag{14}$$

and

$$g^{;\nu}_{;\mu} = g^{;\nu}_{\ ,\mu} + g^{;\nu}A_\mu + A^\dagger_\mu\,g^{;\nu}. \tag{15}$$

In terms of them, the variational equations of the space-time integral of L are:

$$\phi^{;\mu}_{\ ,\mu} + g^{-1}g_{,\mu}\,\phi^{,\mu} = 0 \tag{16}$$

$$F^{\mu\nu}_{\ \ ;\nu} = [F^{\mu\nu}, g^{-1}g_{;\nu}] - \tfrac{1}{2}e^2m^2g^{-1}g^{;\mu} \tag{17}$$

$$g^{\ \mu}_{;\mu} = g_{;\mu}\,g^{-1}g^{;\mu} + e^{-2}m^{-2}g[g^{-1}F^\dagger_{\mu\nu}\,g, F^{\mu\nu}] + 2m^{-2}\,g\phi^{,\mu}\phi^\dagger_{,\mu}\,g\,. \tag{18}$$

The $\mu = 0$ component of the equation for $F^{\mu\nu}$ is a constraint, which may be called Gauss's law. By using it, one may identify the Hamiltonian density as

$$H = \phi^\dagger_{,\mu}g\phi_{,\mu} + \tfrac{1}{4}m^2\,\mathrm{tr}[(g_{;\mu}\,g^{-1})^2] + \tfrac{1}{2}e^{-2}\mathrm{tr}(F^\dagger_{\mu\nu}\,gF_{\mu\nu}\,g^{-1}) \tag{19}$$

in which each term is positive as long as g is positive.

The antisymmetry of $F^{\mu\nu}$ implies that the $n\times n$ matrix of currents

$$j^\mu = [F^{\mu\nu}, g^{-1}g_{;\nu} - A_\nu] - \tfrac{1}{2}e^2m^2\,g^{-1}g^{;\mu} \tag{20}$$

is conserved, $j^\mu_{\ ,\mu} = 0$. By combining this conservation law with the field equation for g, one may derive the constraint

$$\phi^*_{i,\mu}\,\phi^{;\mu}_{j} = 0 \tag{21}$$

for all i, j, and x.

A special class of simple solutions of the field equations (16)–(18) is given by the choice $g = 1$, $A_\mu = 0$, and $\phi_i(x) = f_i(k_i\cdot x)$ where the f's are arbitrary functions and the k's form a set of colinear null vectors, $k_i\cdot k_j = 0$. None of these solutions has finite energy, except the choice $k_i = 0$ for all i. The superposition of two such special solutions is not in general a solution since the constraint (21) is nonlinear.

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U(N) integral for the generating functional in lattice gauge theory [a)]

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The one link integral or equivalently the generating functional of U(N) integrals in the lattice gauge theory is explicitly evaluated in terms of a character expansion.

In U(N) lattice gauge theories[1] and also in the lattice version of the nonlinear U(N)×U(N) sigma model one encounters certain U(N) group integrals. Various approaches have been suggested[2–4] to evaluate such integrals but they all are limited by their perturbative nature. The iterative procedures by which these integrals are usually evaluated have been carried out in practice only up to a few orders. Here the complete answer for any N is provided in the form of a character expansion of the generating function of the desired integrals. Any lattice integral can be evaluated by taking derivatives of the generating function which is given explicitly in this paper.

The generating functional for the lattice gauge theory (or sigma model) has the form

$$\int [dU]\, e^{-S(U)/g^2 + \Sigma \mathrm{Tr}(KU + U^\dagger K^\dagger)}, \tag{1}$$

where S is the action, U is the unitary group element of U(N) associated with each link (or corner) of the lattice, K is the source term associated with each link (or corner) and dU is the Haar measure for the group U(N) for each link (or corner). Any Green's function or correlation function, such as the Wilson loop,[1] is obtained from Eq. (1) by differentiating with respect to K and $K^\dagger$ independently, so as to bring down the appropriate factors of U's and then setting $K = 0 = K^\dagger$. Equation (1) may be rewritten as

$$e^{-S(\delta/\delta K)/g^2} \int dU\, e^{\mathrm{Tr}(KU + U^\dagger K^\dagger)}, \tag{2}$$

where every U in the action has been replaced by the functional derivative $\delta/\delta K$ of the corresponding link. Note that the remaining integrals over the individual links are decoupled from each other. In the strong coupling limit one may expand $e^{S(\delta/\delta K)/g^2}$ in powers of $(1/g^2)$ and evaluate the interaction between links perturbatively by taking derivatives. Then at various orders one would have to evaluate certain U(N) integrals. Thus we see that the generating functional for the desired integrals is simply

$$\int dU\, e^{\mathrm{Tr}(KU + U^\dagger K^\dagger)} \tag{3}$$

for any given link. The integral for $K \neq 0$ but $K^\dagger = 0$ was evaluated in Ref. 2 but this is not sufficient.

This same integral occurs in a different context if one attempts a link by link integration[4] of the lattice theory in the absence of sources. Concentrating on one link, the integral to be performed has the form[4]

$$\int dU\, e^{\mathrm{Tr}(UA + A^\dagger U^\dagger)/g^2}, \tag{4}$$

where $A = \Sigma_i U_i$ is the sum of unitary matrices that complete the neighboring plaquettes that couple to the link U.

In this paper some powerful group theoretical methods will be used to evaluate the generating functional

$$Z_N(J,J^\dagger) = \int dU\, e^{\beta N \mathrm{tr}(JU + U^\dagger J^\dagger)} \tag{5}$$

as a function of arbitrary sources J and $J^\dagger$. The two situations described above will be covered by taking the appropriate values of $\beta NJ = K$ or $\beta NJ = A/g^2$. The factor of N is included to prepare the grounds for analyzing the $N \to \infty$ of Eq. (4).

Consider an arbitrary group element g of the general linear group GL(N) in the $N \times N$ fundamental representation. The function exp(Trg) is invariant under the group and, therefore, has an expansion in terms of the characters $\chi_r(g)$ of GL(N)

$$e^{\beta N \mathrm{Tr} g} = \sum_r a_r(\beta N)\chi_r(g), \tag{6}$$

where the sum is over all representations of the group. The coefficients $a_r(\beta N)$ are to be determined. This expansion is a generalization of the familiar Legendre polynomial expansion of a rotationally invariant function which diagonalizes angular momentum. Inserting this form into the integral and identifying $g = JU$ and $g^\dagger = U^\dagger J^\dagger$ one obtains

$$Z_N(J,J^\dagger) = \sum_{r,r'} a_r a_{r'} \int dU \chi_r(JU)\chi_{r'}(U^\dagger J^\dagger). \tag{7}$$

The U(N) integral over the characters is well known to give

$$\int dU\, \chi_r(JU)\chi_{r'}(U^\dagger J^\dagger) = \delta_{rr'} \frac{\chi_r(JJ^\dagger)}{d_r}, \tag{8}$$

where $d_r = \chi_r(1)$ is the dimension of the representation. Thus, the final form is

$$Z_N(JJ^\dagger) = \sum_r a_r^2 \frac{\chi_r(JJ^\dagger)}{d_r}. \tag{9}$$

Note that the result is a group invariant function of the matrix $JJ^\dagger$ which may be considered a group element of GL(N) in the fundamental $N \times N$ representation.

There remains now to calculate the coefficients a_r and to write more explicitly the characters $\chi_r(g)$. Let us first evaluate a_r. Equation (6) can be specialized to the unitary subgroup U(N) of GL(N) without changing the coefficients

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a_r. Then one has

$$e^{\beta N \operatorname{Tr} U} = \sum_r a_r \chi_r(U). \tag{10}$$

Using the orthogonality property of characters [Eq. (8)] this equation may be inverted in the form

$$a_r(\beta N) = \int dU \chi_r(U^\dagger) e^{\beta N \operatorname{Tr} U}. \tag{11}$$

Now, since the measure of integration dU is the Haar measure which is invariant under both left and right transformations, one can diagonalize $U = T\lambda T^{-1}$ inside the integral. The T integration can be done trivially since the integrand is independent of T. Therefore, one remains with the integral over the eigenvalues $\lambda_k = e^{i\phi_k}$, $0 \leqslant \phi_k \leqslant 2\pi$, of the matrix U:

$$a_r(\beta N) = \int d\mu(\phi) \chi_r^*(\phi) e^{\beta N (e^{i\phi_1} + e^{i\phi_2} + \cdots + e^{i\phi_N})}. \tag{12}$$

The representation r of U(N) can be labeled by N integers $r = (n_1, n_2, \ldots, n_N)$ with $n_1 \geqslant n_2 \geqslant \ldots \geqslant n_N$, where n_i correspond to the number of boxes in the ith row of a Young tableau. The measure $d\mu(\phi)$ and the character $\chi_r(\phi)$ in terms of the angles ϕ_k have both been given by Weyl[5]:

$$\begin{aligned} d\mu(\phi) &= \frac{d\phi_1}{2\pi} \cdots \frac{d\phi_N}{2\pi} \Delta(\phi) \Delta^*(\phi), \\ \Delta(\phi) &= (1/\sqrt{N!}) \det[e^{i(N-j)\phi_k}], \\ \Delta^*(\phi) \chi^*_{(n_1, n_2, \ldots, n_N)} &= (1/\sqrt{N!}) \det[e^{-i(N-j+n_j)\phi_k}], \end{aligned} \tag{13}$$

where the quantities inside the "det" are to be viewed as the (jk) element of a matrix M_{jk}. Then one arrives at

$$\begin{aligned} a_{(n_1, \ldots n_N)} &= \frac{1}{N!} \epsilon_{i_1 \ldots i_N} \epsilon_{j_1 \ldots j_N} \\ &\quad \times \prod_{k=1}^{N} \int_0^{2\pi} \frac{d\phi_k}{2\pi} e^{-i\phi_k (n_{i_k} + j_k - i_k)} e^{\beta N e^{i\phi_k}} \\ &= \det\left(\frac{1}{(n_i + j - i)!}\right) \times (\beta N)^{n_1 + n_2 + \cdots + n_N} \\ &= \begin{vmatrix} \frac{1}{n_1!} & \frac{1}{(n_1+1)!} & \cdots & \frac{1}{(n_1+N-1)!} \\ \frac{1}{(n_2-1)!} & \frac{1}{n_2!} & \cdots & \frac{1}{(n_2+N-2)!} \\ \frac{1}{(n_N-N+1)!} & \cdots & \cdots & \frac{1}{n_N!} \end{vmatrix} \\ &\quad \times (\beta N)^{n_1 + n_2 + \cdots + n_N}. \end{aligned} \tag{14}$$

The determinant can be evaluated explicitly, and it takes the following various forms:

$$\begin{aligned} &\det\left(\frac{1}{(n_i + j - i)!}\right) \\ &= \frac{1}{n_1! n_2! \cdots n_N!} \prod_{1 \leqslant i < j \leqslant N} \left(1 - \frac{n_j}{n_i + j - i}\right) \\ &= d_{(n_1, n_2, \ldots n_N)} \prod_{i=1}^{N} \frac{(N-i)!}{(n_i + N - i)!}, \end{aligned} \tag{15}$$

where $d_{(n_1, \ldots, n_N)}$ is the dimension of the representation $(n_1, \ldots, n_N)$

$$d(n_1, \ldots, n_N) = \prod_{1 \leqslant i < j \leqslant N} \left(1 + \frac{n_i - n_j}{j - i}\right). \tag{16}$$

Replacing this result in Eq. (9) one arrives at

$$\begin{aligned} Z_N(JJ^\dagger) = \sum_{n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0} &\left\{ \frac{(\beta^2 N^2)^{n_1 + n_2 + \cdots + n_N}}{(n_1!)^2 (n_2!)^2 \cdots (n_N!)^2} \right. \\ &\times \prod_{1 \leqslant i < j \leqslant N} \left(1 - \frac{n_j}{n_i + j - i}\right)^2 \\ &\left. \times \frac{\chi_{(n_1, n_2, \ldots n_N)}(JJ^\dagger)}{d_{(n_1, n_2, \ldots n_N)}} \right\}. \end{aligned} \tag{17}$$

Note that each term in this sum is positive. The denominator never vanishes, therefore, there can be no de Wit–'t Hooft poles.[6]

The character $\chi_r(JJ^\dagger)$ can be explicitly given in various forms. One formula has already been indicated in Eq. (13) except that instead of the phases $e^{i\phi_k}$ we need to replace the eigenvalues λ_k of the Hermitian matrix $JJ^\dagger$. However, in physical applications one needs the explicit dependence on the matrix $H = JJ^\dagger$ rather than on its eigenvalues. Such a form is also available in the literature[5] and can be given as follows[7]: Let the character corresponding to the single row Young tableau with n boxes be denoted by $\chi_n(H)$:

$$\chi_n(H) = \chi_{(n,0,0,\ldots 0)}(H). \tag{18}$$

Then $\chi_n(H)$ can be computed from

$$\chi_n(H) = \int_0^{2\pi} \frac{d\phi}{2\pi} \frac{e^{-in\phi}}{\det(1 - e^{i\phi} H)} \tag{19}$$

which yields

$$\begin{aligned} \chi_n(H) &= \sum_{k_1, \ldots, k_N} \left(\frac{\operatorname{Tr} H}{1}\right)^{k_1} \left(\operatorname{Tr} \frac{H^2}{2}\right)^{k_2} \cdots \left(\operatorname{Tr} \frac{H^n}{n}\right)^{k_n} \\ &\quad \times \frac{\delta(k_1 + 2k_2 + \cdots + nk_n - n)}{k_1! k_2! \cdots k_n!} \\ &= \frac{(\operatorname{Tr} H)^n}{n!} + \frac{(\operatorname{Tr} H)^{n-2}}{(n-2)!} \operatorname{Tr} \frac{H^2}{2} \\ &\quad + \frac{(\operatorname{Tr} H)^{n-3}}{(n-3)!} \operatorname{Tr} \frac{H^3}{3} + \cdots + \operatorname{Tr} \frac{H^n}{n}. \end{aligned} \tag{20}$$

The general character $\chi_{(n_1, n_2, \ldots, n_N)}$ is then given in terms of $\chi_n(H)$ as a determinant[5,7]

$$\chi_{(n_1, n_2, \cdots, n_N)} = \begin{vmatrix} \chi_{n_1} & \chi_{n_2 - 1} & \cdots & \chi_{n_N - N + 1} \\ \chi_{n_1 + 1} & \chi_{n_2} & \cdots & \chi_{n_N - N + 2} \\ \cdots & \cdots & & \cdots \\ \chi_{n_1 + N - 1} & \chi_{n_2 + N - 2} & \cdots & \chi_{n_N} \end{vmatrix}, \tag{21}$$

where one used the convention that $\chi_0 = 1$ and $\chi_n = 0$ if n is a negative integer. Note that according to that convention the rank of the determinant reduces to the number of nontrivial rows in a given Young tableau. For illustration, a list of

TABLE I. List of characters and dimensions.

$$\chi_{(1,0,\dots)} = \mathrm{Tr}H$$

$$d_{(1,0,\dots)} = N$$

$$\chi_{(2,0,\dots)} = \frac{1}{2!}[(\mathrm{Tr}H)^2 + \mathrm{Tr}H^2]$$

$$d_{(2,0,\dots)} = \frac{1}{2}N(N+1)$$

$$\chi_{(1,1,0,\dots)} = \frac{1}{2!}[(\mathrm{Tr}H)^2 - \mathrm{Tr}H^2]$$

$$d_{(1,1,0,\dots)} = \frac{1}{2}N(N-1)$$

$$\chi_{(3,0,0,\dots)} = \frac{1}{3!}[(\mathrm{Tr}H)^3 + 3\mathrm{Tr}H\,\mathrm{Tr}H^2 + 2\mathrm{Tr}H^3]$$

$$d_{(3,0,0,\dots)} = \frac{1}{3!}N(N+1)(N+2)$$

$$\chi_{(2,1,0,\dots)} = \frac{1}{3}[(\mathrm{Tr}H)^3 - \mathrm{Tr}H^3]$$

$$d_{(2,1,0,\dots)} = \frac{1}{3}(N-1)N(N+1)$$

$$\chi_{(1,1,1,0,\dots)} = \frac{1}{3!}[(\mathrm{Tr}H)^3 - 3\mathrm{Tr}H\,\mathrm{Tr}H^2 + 2\mathrm{Tr}H^2]$$

$$d_{(1,1,1,0,\dots)} = \frac{1}{3!}(N-2)(N-1)N$$

$$\chi_{(4,0,0,0,\dots)} = \frac{1}{4!}[(\mathrm{Tr}H)^4 + 6(\mathrm{Tr}H)^2\mathrm{Tr}H^2 + 8\mathrm{Tr}H\,\mathrm{Tr}H^3 + 3(\mathrm{Tr}H^2)^2 + 6\mathrm{Tr}H^4]$$

$$d_{(4,0,0,0,\dots)} = \frac{1}{4!}N(N+1)(N+2)(N+3)$$

$$\chi_{(3,1,0,0,\dots)} = \frac{1}{8}[(\mathrm{Tr}H)^4 + 2(\mathrm{Tr}H)^2\mathrm{Tr}H^2 - (\mathrm{Tr}H^2)^2 - 2\mathrm{Tr}H^4]$$

$$d_{(3,1,0,0,\dots)} = \frac{1}{8}(N-1)N(N+1)(N+2)$$

$$\chi_{(2,2,0,0,\dots)} = \frac{1}{12}[(\mathrm{Tr}H)^4 - 4\mathrm{Tr}H\,\mathrm{Tr}H^3 + 3(\mathrm{Tr}H^2)^2]$$

$$d_{(2,2,0,0,\dots)} = \frac{1}{12}(N-1)N^2(N+1)$$

$$\chi_{(2,1,1,0,\dots)} = \frac{1}{8}[(\mathrm{Tr}H)^4 - 2(\mathrm{Tr}H)^2\mathrm{Tr}H^2 - (\mathrm{Tr}H^2)^2 + 2\mathrm{Tr}H^4]$$

$$d_{(2,1,1,0,\dots)} = \frac{1}{8}(N-2)(N-1)N(N+1)$$

$$\chi_{(1,1,1,1,0,\dots)} = \frac{1}{4!}[(\mathrm{Tr}H)^4 - 6(\mathrm{Tr}H)^2\mathrm{Tr}H^2 + 8\mathrm{Tr}H\,\mathrm{Tr}H^3 + 3(\mathrm{Tr}H^2)^2 - 6\mathrm{Tr}H^4]$$

$$d_{(1,1,1,1,0,\dots)} = \frac{1}{4!}(N-3)(N-2)(N-1)N$$

characters is given explicitly in Table I which are in accordance with these general formulas. They can be used to rewrite the result in terms of the invariants $\mathrm{Tr}(JJ^\dagger)^k$. It can be checked then that the present general result agrees with previous limited calculations.[2–4]

It is also useful to calculate $W_N(JJ^\dagger)$ which is the generating functional for connected graphs. It is defined by

$$Z_N(JJ^\dagger) = \int dU\, e^{\beta N \mathrm{Tr}(JU + U^\dagger J^\dagger)} = e^{N^2 W_N(JJ^\dagger)}, \tag{22}$$

where the extra factor of N^2 in the exponent is inserted for convenience. Thus, $W_N(JJ^\dagger)$ can be calculated by taking the logarithm of $Z_N(JJ^\dagger)$in Eq. (17):

$$W_N(JJ^\dagger) = (1/N^2)\ln Z_N(JJ^\dagger). \tag{23}$$

The logarithm cannot be evaluated in closed form. One may attempt a series expansion in powers of β. It is convenient to express the answer in terms of the invariants x_k defined below

$$x_1 = \frac{1}{N}\mathrm{Tr}JJ^\dagger,$$

$$x_k = \frac{1}{N}\mathrm{Tr}\left(JJ^\dagger - \mathbb{1}\frac{\mathrm{Tr}JJ^\dagger}{N}\right)^k, \quad 2 \leqslant k \leqslant N, \tag{24}$$

where $JJ^\dagger - \mathbb{1}\mathrm{Tr}JJ^\dagger/N$ is traceless. These are all the N invariants that can be formed from the GL(N) matrix $JJ^\dagger$, so that the result can always be expressed in terms of these N variables and their powers. The expansion up to β^{10} yields

$$\begin{aligned} W_N(JJ^\dagger) &= \beta^2 x_1 - \frac{1/2\beta^4 x_2}{(1-1/N^2)} + \frac{2/3\beta^6 x_3}{(1-1/N^2)(1-4/N^2)} \\ &- \frac{5/4\beta^8 x_4}{(1-1/N^2)(1-4/N^2)(1-9/N^2)} \\ &+ \frac{3/4(3-7/N^2)\beta^8 (x_2)^2}{(1-1/N^2)^2(1-4/N^2)(1-9/N^2)} \\ &+ \frac{14/5\beta^{10}x_5}{(1-1/N^2)(1-4/N^2)(1-9/N^2)(1-16/N^2)} \\ &- \frac{4(3-13/N^2)\beta^{10}x_2x_3}{(1-1/N^2)^2(1-4/N^2)(1-9/N^2)(1-16/N^2)} \\ &- \frac{7\beta^{12}x_6}{(1-1/N^2)\cdots(1-25/N^2)} + \cdots \end{aligned} \tag{25}$$

From this expression a trend can be seen so that the coefficient of x_k for $k \geqslant 1$ can be guessed as

$$\frac{(1/2k)\binom{1/2}{k}(2\beta)^{2k}x_k}{(1-1/N^2)\cdots(1-(k-1)^2/N^2)}, \quad 1 \leqslant k \leqslant N. \tag{26}$$

For $k > N$ it is necessary to consider terms in the form of products of the x_k such as x_1^N, $x_N x_1$, $x_N x_2$, etc. since the powers $\mathrm{Tr}(JJ^\dagger)^k$ for $k > N$ can always be rewritten in terms of the x_k. However, if one wishes, the answer could also be given in terms of higher powers. The general coefficients for the products of x_k's analogous to $(x_2)^2$, x_2x_3, etc., have not yet been obtained.

One may take Eq. (26) as an indication of the convergence properties of the series expansion of $W_N(JJ^\dagger)$ and analyze the $N\to\infty$ limit. First, note that the de Wit–'t Hooft poles are illusory as already noted following Eq. (17). Therefore, to get a feeling of the convergence properties, let us approximate the denominator in Eq. (26) by 1 and extend its validity up to $k\to\infty$. Second, note that in the approach of Ref. 4 and Eq. (4), J is bounded by the number of dimensions of the lattice. In d-dimensions each link has $2(d-1)$ neighbors, so that $J \lesssim 2(d-1)$. Thus,

$$x_k \lesssim (2(d-1))^{2k} \tag{27}$$

is a generous bound considering that x_k is defined in terms of the traceless part of $JJ^\dagger$. Thus, we may conclude that the

series converges for

$$2\beta \times 2(d-1) \lesssim 1. \tag{28}$$

Therefore, for sufficiently small β ($\beta < 1/4(d-1)$), the series can be approximated by its first term

$$W_N(JJ^\dagger) \approx (\beta^2/N)\mathrm{Tr}(JJ^\dagger). \tag{29}$$

The consequences of such an approximation have already been discussed in Ref. (4) and shown to lead to a latticized string theory. While it appears that this approximation does not reproduce certain diagrams which survive the usual large N limit[8] it must be that such diagrams are small dynamically in the limit indicated here (β = small). We must emphasize that this is not an approximation based on an expansion parameter but also on the structure of the integrals that occur in the theory. Furthermore, as emphasized in Ref. (4), the emerging string picture corresponds to the strong coupling limit and hence to the large distance behavior of the theory. The string result should *not* be extrapolated naively to the continuum weak coupling limit of QCD. In fact, the possibility of phase transitions in the $N\to\infty$ limit has been raised[9] so that the weak coupling behavior of the theory will need a different treatment.

The $N\to\infty$ phase transition found by Gross and Witten in two-dimensions can be seen in our approach as follows: Set $J = 1$ then one has $x_1 = 1$, $x_k = 0$ for $k \geqslant 2$. This yields via Eqs. (24)–(26)

$$W_N(1) = \beta^2 + C_{N+1}(4\beta^2)^{N+1} + \cdots, \tag{30}$$

where the terms of order $N+1$ come from terms $k = N+1$ which involve the power x_1^{N+1}. There will be nonvanishing terms only for $(4\beta^2)^{nN+1}$ according to the trend established in Eqs. (25) and (26). Now one can see that as $N\to\infty$ all higher order terms vanish exponentially if $\beta < 1/2$, so that $W_N(1) = \beta^2$ becomes an *exact* result. For $\beta > 1/2$ the higher order terms take over and one has to sum the series before evaluating $W_N(1)$, which would certainly be different than β^2, as shown in Ref. 9 via other methods.

There is one case for which it is possible to obtain an exact answer in the $N\to\infty$ limit with the formulas presented so far. This occurs when x_k is of order $1/N$ for all k as it would be, for example, if J is of the form[4] $J = \mathrm{diag.}(1,0,0,\ldots)$ or many other nontrivial examples. Then in Eq. (25) we need to retain only the terms which are of first power in the various x_k. However, such terms are exactly those given in Eq. (26) and they sum to

$$\begin{aligned} W_N &= \sum_{k=1}^{\infty} \frac{1}{2k}\binom{\frac{1}{2}}{k}(2\beta)^{2k}\frac{\mathrm{Tr}(JJ^\dagger)^k}{N} + 0(1/N^2) \\ &= \frac{1}{N}\mathrm{Tr}[(1+4\beta^2 JJ^\dagger)^{1/2} - 1 \\ &\quad - \ln(\tfrac{1}{2} + \tfrac{1}{2}(1+4\beta^2 JJ^\dagger)^{1/2})] + 0(1/N^2). \end{aligned}$$

We do not know of a direct application of this result in the lattice theory.

It would clearly be valuable to complete the calculation of $W_N(JJ^\dagger)$ for $(1/N)\mathrm{Tr}JJ^\dagger$ = finite, or to directly manipulate our exact result for $Z_N(JJ^\dagger)$ in order to analyze the weak coupling limit of the lattice theory.

After the completion of the present work I was informed of another independent attempt by S. Samuels to calculate certain group integrals exactly. His methods and the form of his results are rather different than ours.[10]

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Poincaré wave equations as Fourier transforms of Galilei wave equations

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The relationship between the Poincaré and Galilei groups allows us to write the Poincaré wave equations for arbitrary spin as a Fourier fransform of the Galilean ones. The relation between the Lagrangian formulation for both cases is also studied.

I. INTRODUCTION

It is well known that the Galilei algebra is a subalgebra of Poincaré algebra in one space dimension more.[1] This fact allows us to relate relativistic Poincaré and Galilean theories. An interesting point is that Galilei transformations in two space dimensions are contained in the usual Poincaré transformations.[2] This enables us to present Poincaré spin zero wavefunctions as Fourier transforms of Galilean ones. In the same way it is possible to see the Klein–Gordon equation as the Fourier transform of the Schrödinger equation in one space dimension less.

On the other hand, due to the fact that the Poincaré algebra is a subalgebra of the complex Galilei algebra in one space dimension more,[3] it is possible to do a similar analysis as in the preceding case, i.e., the Schrödinger equation can be obtained as a Fourier transform of the Klein–Gordon equation.[2]

The aim of this paper is to extend the results above quoted to the arbitrary spin case and study the possible relations between the Lagrangian formulations of Poincaré and Galilei theories.

The organization of this paper is as follows: In Sec. 2 we give a summary of the results of Ref. 2, in Sec. 3 we extend these results to the arbitrary spin case; in Sec. 4 we study some aspects of the Lagrangian formulation; Sec. 5 is devoted to conclusions.

II. POINCARÉ AND GALILEI SPIN-0 WAVE EQUATIONS

The light cone transformation

$$t = \frac{1}{\sqrt{2}}(x^0 - x^3), \quad x = x^1, \quad y = x^2,$$
$$s = \frac{1}{\sqrt{2}}(x^0 + x^3), \tag{2.1}$$

induces[1] the (2 +1) Galilei algebra

$$J = J_3, \quad \mathscr{P}_1 = P_1, \quad \mathscr{P}_2 = P_2,$$
$$G_1 = \frac{1}{\sqrt{2}}(K_1 + J_2), \quad G_2 = \frac{1}{\sqrt{2}}(K_2 - J_1), \tag{2.2}$$
$$\mathscr{H} = \frac{1}{\sqrt{2}}(P_0 - P_3), \quad M = \frac{1}{\sqrt{2}}(P_0 + P_3),$$

where P_μ, **J**, and **K** are the generators of the (3 +1) Poincaré algebra.

If we take the linearized natural representation of the Poincaré group acting on $(x^0, x^1, x^2, x^3, 1)$ and subduce it to the Galilei subgroup generated by (2.2), we obtain, in the coordinates (2.1), the transformation

$$t' = t + b, \quad x_\perp' = Rx_\perp + v_\perp t + a_\perp,$$
$$\left[x_\perp \equiv \begin{pmatrix} x \\ y \end{pmatrix}\right], \quad s' = s + v_\perp x_\perp + \tfrac{1}{2}v_\perp^2 t + \theta, \tag{2.3}$$

which is the natural representation of the (2 +1) extended Galilei group.

Notice that the s transformation is related to the phase that appears in the projective representations of the Galilei group.[4]

Let us now relate the spin-0 Poincaré and Galilei wave functions by means of a Fourier transformation. A wavefunction $\psi(t, x_\perp, s)$ scalar under Poincaré group can be expressed as

$$\psi(t, x_\perp, s) = \int d\eta\, e^{-i\eta s}\phi_\eta(t, x_\perp), \tag{2.4}$$

where $\phi_\eta(t, x_\perp)$ is a scalar wavefunction under the (2 +1) extended Galilei group. Now we can write the Klein–Gordon equation as

$$(\Box + m^2)\psi(t, x_\perp, s) = \int d\eta\, e^{-i\eta s}(S\phi_\eta)(t, x_\perp), \tag{2.5}$$

where $(S\phi_\eta)$ is the Schrödinger equation for a (2 +1) Galilean particle of mass η.

On the other hand, the imaginary coordinate transformation[2]

$$x^0 = iz, \quad x^1 = x, \quad x^2 = y, \quad x^3 = \gamma t, \quad \gamma \text{ arbitrary}, \tag{2.6}$$

induces the (2 +1) Poincaré algebra

$$\mathscr{J} = J_3, \quad K_1 = -iJ_2, \quad K_2 = iJ_1,$$
$$\mathscr{P}_1 = P_1, \quad \mathscr{P}_2 = P_2, \quad \mathscr{H} = -iP_3, \tag{2.7}$$

where **P**, **J** are the generators of translations and rotations of the (3 +1) Galilei group.

As in the preceeding case, if we take the linearized natural representation of the extended Galilei group acting on $(x, y, z, t, s, 1)$ and subduce it to the Poincaré subgroup generated by (2.7), we can obtain, using (2.6), the natural representaiton of the (2 +1) Poincaré group.

A wavefunction $\phi(t, \mathbf{x})$ scalar under Galilei group can be written, using (2.6), as

$$\phi(x^0, x^1, x^2, x^3) = \int d\lambda\, e^{-i\lambda x^3}\psi_\lambda(x^0, x^1, x^2), \tag{2.8}$$

where $\psi_\lambda(x^0, x^1, x^2)$ is a scalar wavefunction under the (2 +1) Poincaré group. In the same way, the Schrödinger

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equation can be written as

$$(S\phi)(x^0, x^1, x^2, x^3) = \int d\lambda\, e^{-i\lambda x^3}(\text{K-G})\psi_\lambda(x^0, x^1, x^2)\,, \tag{2.9}$$

where $(\text{K-G})\psi_\lambda$ is the Klein–Gordon equation in $(2+1)$ dimensions with mass $M^2 = -2m\gamma\lambda$.

Let us remark that the invariance of the Klein–Gordon equation implies, by (2.5), the invariance of the Schrödinger equation. Due to (2.9), the inverse is also true.

III. POINCARE AND GALILEI SPIN S WAVE EQUATIONS

We shall first concentrate ourselves in the Dirac equation for a spin $\frac{1}{2}$ particle of mass m. This equation is invariant under the $\mathscr{D} \equiv D^{(1/2,0)\otimes(0,1/2)}$ representation of $SL(2,C)$ with generators

$$\mathbf{J} = \tfrac{1}{2}\begin{pmatrix}\bar{\boldsymbol{\sigma}} & 0\\ 0 & \bar{\boldsymbol{\sigma}}\end{pmatrix}, \quad \bar{\mathbf{K}} = \frac{i}{2}\begin{pmatrix}\bar{\boldsymbol{\sigma}} & 0\\ 0 & \bar{\boldsymbol{\sigma}}\end{pmatrix}. \tag{3.1}$$

If this representation is subduced using (2.2), to the $(2+1)$ Galilei algebra, we obtain an equivalent representation of that of Levy-Leblond[4] for spin $\frac{1}{2}$.

This equivalence can be expressed by a matrix A, whose explicit form is given by

$$A = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & 0 & 0 & -i\\ 0 & 0 & \dfrac{1}{\sqrt{2}} & 0\\ 0 & \dfrac{-i}{\sqrt{2}} & 0 & 0\end{pmatrix}. \tag{3.2}$$

Using this matrix, we obtain

$$\tilde{J} = AJA^{-1} = \tfrac{1}{2}\begin{pmatrix}\sigma_3 & 0\\ 0 & \sigma_3\end{pmatrix},$$
$$\tilde{G} = AG_iA^{-1} = \tfrac{1}{2}\begin{pmatrix}0 & 0\\ \sigma_i & 0\end{pmatrix}, \quad i = 1, 2\,, \tag{3.3}$$

which is the usual representation of the Galilei algebra.

The matrix A acts on Dirac spinors: $\psi^A_{\mathrm{D}} = A\psi_{\mathrm{D}}$. Now we can generalize (2.4), writing

$$\psi^A_{\mathrm{D}}(t, x_\perp, s) = \int d\eta e^{-i\eta s}\phi_{\eta\mathrm{LL}}(t, x_\perp)\,, \tag{3.4}$$

where $\phi_{\eta\mathrm{LL}}$ is a Galilean wavefunction for a spin $\frac{1}{2}$ particle of mass η, and now we can write the Dirac equation for ψ^A_{D} as

$$A(\gamma_\mu P^\mu - m)A^{-1}\psi^A_{\mathrm{D}}(t, x_\perp, s) = \int d\eta\, e^{-i\eta s}G_\eta\phi_{\eta\mathrm{LL}}(t, x_\perp)\,, \tag{3.5}$$

where

$$G_\eta\phi_{\eta\mathrm{LL}} = \begin{pmatrix}-i\sigma_\perp P_\perp - m & 2\eta\\ E & i\sigma_\perp P_\perp - m\end{pmatrix}\begin{pmatrix}\varphi_\eta\\ \chi_\eta\end{pmatrix}, \tag{3.6}$$

is the Levy-Leblond equation in $(2+1)$ dimensions for a particle of mass η and spin $\frac{1}{2}$. Therefore, the Dirac equation is the Fourier transform of Levy-Leblond equations.

Let us search the transformations properties of the Galilean spinor $\phi_{\eta\mathrm{LL}}$ from those of the corresponding Dirac spinor.

Under the Lorentz group, the Dirac spinor transforms as

$$\psi'_{\mathrm{D}}(x') = \mathscr{D}(\Lambda)\psi_{\mathrm{D}}(x)\,.$$

If we restrict ourselves to transformations belonging to the $(2+1)$ homogeneous Galilei group, $\Lambda = \Lambda_{\mathrm{G}}$, the new Dirac spinor ψ^A_{D} transforms as

$$\psi'^A_{\mathrm{D}}(t', x'_\perp, s') = \Delta(\Lambda_{\mathrm{G}})\psi^A_{\mathrm{D}}(t, x_\perp, s)\,, \tag{3.7}$$

where $\Delta(\Lambda_{\mathrm{G}}) = A\mathscr{D}(\Lambda_{\mathrm{G}})A^{-1}$ is the $(2+1)$ Galilei subduced representation generated by (3.3).

Using (3.4), (3.7) is given by

$$\int d\eta\, e^{-i\eta s'}\phi'_{\eta\mathrm{LL}}(t' x'_\perp) = \Delta(\Lambda_{\mathrm{G}})\int d\eta\, e^{-i\eta s}\phi_{\eta\mathrm{LL}}(t, x_\perp)\,,$$

and from (2.3) we have

$$\phi'_{\eta\mathrm{LL}}(t', x'_\perp) = e^{if}\Delta(\Lambda_G)\phi_{\eta\mathrm{LL}}(t, x_\perp)\,, \tag{3.8}$$

where $f = [v_\perp x_\perp + \frac{1}{2}v_\perp{}^2 t\,]\eta$ is the known phase which appears in the projective representations of the Galilei group.[4]

Now let us note that the operator (3.6) can be put in a more standard form. In order to eliminate the m-dependence we can define a new transformation on the spinors

$$\begin{pmatrix}\hat{\varphi}_\eta\\ \hat{\chi}_\eta\end{pmatrix} = e^{i(m^2/2\eta)t}\begin{pmatrix}I & 0\\ -\dfrac{m}{2\eta} & I\end{pmatrix}\begin{pmatrix}\varphi_\eta\\ \chi_\eta\end{pmatrix},$$

that induces a transformation of the operator (3.6), which becomes

$$\begin{pmatrix}-i\sigma_\perp P_\perp & 2\eta\\ E & i\sigma_\perp P_\perp\end{pmatrix}, \tag{3.9}$$

with a further change (3.9) takes the form

$$\begin{pmatrix}1 & 0\\ 0 & -i\end{pmatrix}\begin{pmatrix}-i\sigma_\perp P_\perp & 2\eta\\ E & i\sigma_\perp P_\perp\end{pmatrix}\begin{pmatrix}i & 0\\ 0 & 1\end{pmatrix} = \begin{pmatrix}\sigma_\perp P_\perp & 2\eta\\ E & \sigma_\perp P_\perp\end{pmatrix}. \tag{3.10}$$

Thus we have obtained the well-known classical form of the Levy-Leblond operator.

It is important to observe that while the operator of (3.9) is invariant under the $(2+1)$ Galilei group due to the invariance of the Dirac operator and the relation (3.5), the Levy-Leblond operator (3.10) is not an invariant one.[5,6]

We can generalize this result to an arbitrary spin case. Let us begin with the Bargmann–Wigner[7] procedure. The Bargmann–Wigner equations are

$$(I \otimes \cdots \otimes \underset{(i)}{D} \otimes \cdots \otimes I)\psi_{\mathrm{BW}}(x^\mu) = 0\,, \quad i = 1 \cdots 2s\,, \tag{3.11}$$

where D is the Dirac operator and ψ_{BW} is a symetric multispinor of rank $2s$. This equation are invariant under the $\mathscr{D} \otimes \cdots \otimes \mathscr{D}$ representation of $SL(2,C)$. If we subduce this representation, using (2.2), to the $(2+1)$ Galilei group, we obtain:

$$\Delta \otimes \cdots \otimes \Delta \,. \tag{3.12}$$

The matrix A acts on symmetric multispinors $\psi^A_{\rm BW} = A \otimes \cdots \otimes A\psi_{\rm BW}$, and analogoulsy to (3.4) we can write

$$\psi^A_{\rm BW}(t, x_\perp, s) = \int d\eta\, e^{-i\eta s}\phi_{{\rm BW}\eta}(t, x_\perp)\,, \tag{3.13}$$

where $\phi_{{\rm BW}\eta}$ is a Galilean symmetric multispinor of rank $2s$. As in spin $\frac{1}{2}$ case the BW equations for $\psi^A_{\rm BW}$ give

$$A \otimes \cdots \otimes A\,(I \otimes \cdots \otimes \underset{(i)}{D} \otimes \cdots \otimes I)A^{-1} \otimes \cdots \otimes A^{-1}\psi^A_{\rm BW}(t, x_\perp, s)$$
$$= \int d\eta\, e^{-i\eta s}(I \otimes \cdots \otimes \underset{(i)}{G_\eta} \otimes \cdots \otimes I)\phi_{{\rm BW}\eta}(t, x_\perp)\,, \quad i = 1\cdots 2s\,, \tag{3.14}$$

where $(I \otimes \cdots \otimes \underset{(i)}{G_\eta} \otimes \cdots \otimes I)\phi_{{\rm BW}\eta}(t, x_\perp)$ $(i = 1\cdots 2s)$ are the BW Galilean equations in $(2+1)$ dimensions for a particle of spin s and mass η. Therefore, the BW equations are the Fourier transform of BW Galilean equations.

If we used another description for a spin s particle, we can obtain simialar results.For example, if we use the reformulate $(6s+1)$ Hurley theory[8] as a modified BW set,[9] i.e.,

$$(\Gamma \otimes \cdots \otimes \underset{(i)}{D} \otimes \cdots \otimes \Gamma)\psi_{\rm BW}(x^\mu) = 0\,, \quad i = 1\cdots 2s\,, \tag{3.15}$$

where D is the Dirac operator and Γ is the projector $\Gamma = \left(\begin{smallmatrix} I & 0 \\ 0 & 0 \end{smallmatrix}\right)$. $\psi_{\rm BW}$ is a symmetric multispinor of rank $2s$. Due to the fact that Γ commutes with the $\mathscr{D}$ representation, of SL (2.C), these equations are invariant under the tensor product of the $\mathscr{D}$ representation.

If we subduce this representation using (2.2) we obtain the Galilei representation (3.12). As in the usual BW case (3.11), the equations (3.15) for $\psi^A_{\rm BW}$ can be written as

$$A \otimes \cdots \otimes A\,(\Gamma \otimes \cdots \oplus \underset{(i)}{D} \otimes \cdots \otimes \Gamma)A^{-1} \otimes \cdots \otimes A^{-1}\psi^A_{\rm BW}(t, x_\perp, s)$$
$$= \int d\eta\, e^{-i\eta s}(P_+ \otimes \cdots \otimes \underset{(i)}{G_\eta} \otimes \cdots \otimes P_+)\phi_{{\rm BW}\eta}(t, x_\perp)\,, \quad i = 1\cdots 2s\,, \tag{3.16}$$

where $(P_+ \otimes \cdots \otimes \underset{(i)}{G_\eta} \otimes \cdots \otimes P_+)\phi_{{\rm BW}\eta}$ is a Galilean equation in $(2+1)$ dimensions for a particle of spin s and mass η in the $(6s+1)$ theory. P_+ is a projector:

$$P_+ = A\Gamma A^{-1} = \begin{pmatrix} 1 & & \\ & 0 & \\ & & 0 \\ & & & 1 \end{pmatrix}. \tag{3.17}$$

Equation $(P_+ \otimes \cdots \otimes \underset{(i)}{G_\eta} \otimes \cdots \otimes P_+)\phi_{{\rm BW}\eta} = 0$ is an invariant Galilean equation owing to the fact that

$$\Delta^{\dagger} P_+ \Delta = P_+ \,.$$

Therefore, the Pincaré $(6s+1)$ theory is the Fourier transform of the Galilei $(6s+1)$ theory.

Summing up, we can say that the possible Poincaré multispinor wave equations can be written as Fourier transforms of the Galilean ones. On the other hand, we can span a symmetric multispinor in a basis of SO(3) tensors. Using this fact it is easy to see that the Poincaré tensorial wave equations can be written as Fourier transforms of Galilei tensorial wave equations.

We want to remark, that in this section we have only studied the Poincaré wavefunctions as Fourier transforms of the Galilei ones, a related analysis can be performed in the inverse situation.

IV. POINCARÉ AND GALILEI LAGRANGIANS

The results of the preceeding sections suggest that it must exist a relation between the Poincaré and Galilei Lagrangians. This is due firstly to the fact that Poincaré wavefunctions are a Fourier transform of the Galilei ones and secondly that the Lagrangians are bilinear functions of the fields.

Let us begin this analysis with the scalar case. The Lagrangian for the Klein–Gordon fields is given by

$$\mathscr{L}_{\rm KG}(x^0, \mathbf{x}) = m^2\psi^*\psi + \mathbf{J}_\mu\psi^*\mathbf{J}^\mu\psi\,, \tag{4.1}$$

if we use the coordinate transformation (2.1), (4.1) can be written as

$$\mathscr{L}_{\rm KG}(t, x_\perp, s) = -m^2\psi^*\psi + \partial_s\psi^*\partial_t\psi + \partial_t\psi^*\partial_s\psi - \partial_i\psi^*\partial_i\psi\,. \tag{4.2}$$

Now, using (2.4), we have

$$\int \mathscr{L}_{\rm KG}(t, x_\perp, s)\, ds = \int d\eta\,[-m^2\phi^*_\eta\phi_\eta - i\eta\partial_t(\phi^*_\eta\phi_\eta) + 2i\eta\phi^*_\eta\partial_t\phi_\eta - \partial_t\phi^*_\eta\partial_t\phi_\eta\,]\,. \tag{4.3}$$

Dimensional reasons suggest to redefine the Galilean fields

$$\hat{\phi}_\eta(t, x_\perp) = (2m\eta)^{1/2}\phi_\eta(t, x_\perp)\,. \tag{4.4}$$

Now, (4.3) becomes

$$\int \mathscr{L}_{\rm KG}(t, x_\perp, s)\, ds = \frac{1}{m}\int d\eta\, \mathscr{L}_{{\rm Sch}\eta}(t, x_\perp)\,, \tag{4.5}$$

where $\mathscr{L}_{{\rm Sch}\eta}$ is the usual Schrödinger Lagrangian with an additive term which is physically interpreted as an energy shift. Moreover we can write

$$W_{\rm KG} = \int d\eta\, W_{{\rm Sch}\eta}\,, \tag{4.6}$$

being $W_{\rm KG}$ the action for the Klein–Gordon field, and $W_{{\rm Sch}\eta}$ the action for the Schrödinger field with mass η in $(2+1)$ dimensions.

We want to remark that the relation (4.6) between the actions is not given by a Fourier transform. This means that if we make a variation $\delta W_{\rm KG} = 0$ it does not imply $\delta W_{{\rm Sch}\eta} = 0$, therefore we can not take (4.6) as a starting point in order to relate Poincaré and Galilean theories.

Now let us consider the relativistic Lagrangian for a spin-$\frac{1}{2}$ particle

$$\mathscr{L}_{\rm D}(x^0, \mathbf{x}) = \psi^\dagger\gamma^0(\gamma_\mu P^\mu - m)\psi\,. \tag{4.7}$$

If we write (4.7) in terms of the new Dirac spinor ψ^A, we have

$$\mathscr{L}_{\rm D}(x^0, \mathbf{x}) = \psi^{A\,\dagger}A^{\dagger\,-1}\gamma^0(\gamma_\mu P^\mu - m)A^{-1}\psi^A\,, \tag{4.8}$$

but under the coordinate transformation (2.1), (4.8) becomes

$$\mathscr{L}_{\rm D}(t, x_\perp, s)$$

$$= \sqrt{2}\psi^{A+}\begin{pmatrix} E & i\sigma_\perp P_\perp - m \\ -i\sigma_\perp P_\perp - m & 2M \end{pmatrix}\psi^A , \qquad (4.9)$$

being $E \equiv i\partial/\partial t$ and $M \equiv i\partial/\partial s$.

Using (3.4) and (4.9), we have

$$\int \mathcal{L}_D(t, x_\perp, s)\, ds$$

$$= \sqrt{2}\int d\eta\, \phi_\eta^+ \begin{pmatrix} E & i\sigma_\perp P_\perp - m \\ -i\sigma_\perp P^\perp - m & 2\eta \end{pmatrix}\phi_\eta . \qquad (4.10)$$

In order to cancel the m-dependence in the rhs of (4.10) and also to recover the dimensionality of the Levy-Leblond field we define

$$\hat{\phi}_\eta(t, x_\perp) = \sqrt{m}\, e^{i(m^2/2\eta)t}\begin{pmatrix} I & 0 \\ -\dfrac{m}{2\eta} & I \end{pmatrix}\phi_\eta(t, x_\perp) . \qquad (4.11)$$

Therefore, we have found

$$\int \mathcal{L}_D(t, x_\perp, s)\, ds = (\sqrt{2}/m)\int d\eta \mathcal{L}_{LL\eta}(t, x_\perp) , \qquad (4.12)$$

where $\mathcal{L}_{LL\eta}$ is the well-known Levy-Leblond Lagrangian for a particle of spin $\frac{1}{2}$.

In the same way as in the spin zero case, we also have

$$W_D = \int d\eta\, W_{LL\eta} ,$$

being W_D and $W_{LL\eta}$, the actions for the Dirac and Levy-Leblond fields, respectively. The remarks we have done for the spin-0 case can serve here unaltered.

IV. CONCLUSIONS

Due to the relation between the Poincaré and Galilei groups, the Poincaré and Galilei transformations are seen to be contained one each other in one space dimension more. This fact allows us to write the Poincaré wavefunctions as Fourier transforms of Galilean ones, and also to find the transformation properties of the Galilei wavefunctions under the (2 +1) Galilei group from the transformation properties of Poincaré wavefunctions under the (3 +1) Poincaré group. In particular it is easy to see the projective character of the representations of the (2 +1) dimensional Galilei group. Taking into account these last properties we can write the Poincaré wave equations for arbitrary spin as Fourier transforms of the Galilean ones, so the Dirac equation can be seen as the Fourier transform of the Levy-Leblond equation.

The relation between Poincaré and Galilei wavefunctions allows us to the relate the Lagrangians of the two theories.

The generalization to the higher spin cases, the relation between the energy–momentum tensor of the two theories and the possible introduction of external fields in this framework is under investigation.

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A solution of an inverse-source problem in coherence theory

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An explicit solution is presented for a special case of the problem of determining the cross spectral density of a radiation source from its far-field intensity pattern. The case considered is that of a flat, circular source radiating into a half-space, where the source coherence properties exhibit statistical homogeneity and isotropy. The solution is in the form of a uniformly convergent series of hypergeometric functions that are straightforwardly related to Legendre polynomials.

1. INTRODUCTION

A recent communication[1] discussed the problem of determining the coherence properties of a radiation source from its far-field intensity pattern. In particular, it was shown that the formulation of this problem given by Steinle and Baltes[2] for a flat, circular source whose coherence properties exhibit statistical homogeneity and isotropy has a unique solution; a method of investigation was outlined for obtaining the solution explicitly in a tractable form. In this paper, the desired solution is presented.

2. BACKGROUND AND PROBLEM STATEMENT

Consider a finite, planar radiation source σ with circular boundary of radius a lying in the plane $z = 0$ of some rectangular coordinate system. Letting $\mathbf{r}_1$ and $\mathbf{r}_2$ denote position vectors in this plane, we suppose with Steinle and Baltes[2] that the cross spectral density, $W(\mathbf{r}_1,\mathbf{r}_2;\omega)$, of the source can be represented as

$$W(\mathbf{r}_1,\mathbf{r}_2;\omega) = W^{\infty}(\mathbf{r}_1,\mathbf{r}_2;\omega)T(\mathbf{r}_1)T^*(\mathbf{r}_2), \tag{1}$$

where W^{∞} is the cross spectral density of an infinite planar source coinciding with the plane $z = 0$, and T is the aperture function

$$T(\mathbf{r}) = \begin{cases} 1, & \text{if } \mathbf{r}\in\sigma, \\ 0, & \text{if } \mathbf{r}\notin\sigma. \end{cases} \tag{2}$$

We assume that the fictitious infinite source is statistically homogeneous and isotropic, i.e., W^{∞} depends only on $|\mathbf{r}_1 - \mathbf{r}_2| = r$ and ω. Assume that the source is radiating into the half space $z > 0$, and let $\mathbf{s}$ denote a unit vector making an angle θ with the positive z axis. Finally, let $I_{\omega}(\mathbf{s})$ denote the intensity at frequency ω in the direction $\mathbf{s}$ measured at range R in the far field of the source.

By using a basic result of Steinle and Baltes[2] that expresses the far-field intensity I_{ω} in terms of the source cross spectral density, it was shown[1] that the entire analytic function $G_{\omega}(z,a)$ defined by

$$G_{\omega}(z,a) = \int_0^{\infty} r\,dr\, W^{\infty}(r;\omega)W_a(r)J_0(zr) \tag{3}$$

is related to the far-field intensity through

$$G_{\omega}(\eta,a) = 2\pi R^2 I_{\omega}/(k^2 - \eta^2), \tag{4}$$

where $\eta = k\sin\theta$, $k = \omega/c$ (c is the speed of light), J_0 is the zeroth-order Bessel function of the first kind, z is a complex variable, and $W_a(r)$ is the convolution of the aperture function T, namely,

$$W_a(r) = \int_{z=0} d^2\mathbf{r}'\, T(\mathbf{r}')T(\mathbf{r}' - \mathbf{r}). \tag{5}$$

Notice that W_a depends only on $r = |\mathbf{r}|$ because of the circular source boundary, and that I_{ω} depends only on θ. It follows from Eq. (4) and analytic continuation arguments that $G_{\omega}(z,a)$ is completely determined by the far-field intensity pattern, so that

$$W^{\infty}(r;\omega)W_a(r) = \int_0^{\infty} x\,dx\, G_{\omega}(x,a)J_0(xr), \tag{6}$$

[where x is a real variable and Eq. (6) follows from the Hankel transform inversion theorem) is also completely determined by the far-field intensity pattern.[1]

The problem addressed in this paper is the explicit determination of $W^{\infty}W_a$ in tractable form, given I_{ω} or, what amounts to the same thing, given $G_{\omega}(x,a)$ for $0\leqslant x\leqslant k$. The problem is clearly to analytically continue G_{ω} to the entire positive real axis, but, as has been shown,[1] the standard power series approach to this problem leads to intractable results. Tractable results can, however, be obtained if $G_{\omega}(x,a)$ is expanded in a suitable set of functions, as will be shown in the rest of this paper.

3. THE SOLUTION

The first step is to expand $G_{\omega}(z,a)$ in a series of the functions

$$g_n(z,a) = J_{2n}(2az)/z^2, \tag{7}$$

where J_{2n} is the $2n$th-order Bessel function of the first kind and $n = 1,2,3,\cdots$. From Eq. (3) it follows that G_{ω} is an even function of z. This fact together with the theory of Neumann expansions[3] guarantees that G_{ω} can always be expressed as

$$G_{\omega}(z,a) = 2\sum_{n=1}^{\infty} a_{2n}\frac{J_{2n}(2az)}{z^2} \tag{8}$$

for some set $\{a_{2n}\}$ of constants.

Define the functions

$$w_n(r^2/4a^2) = (1/2n)\,{}_2F_1(-n,n;1;r^2/4a^2), \quad 0\leqslant r\leqslant 2a,$$
$$w_n(r^2/4a^2) = 0, \quad r > 2a, \tag{9}$$

where ${}_2F_1$ is Gauss' hypergeometric function. Then $g_n(x,a)$ (x being a non-negative real variable) and $w_n(r/4a^2)$ are a zero-order Hankel transform pair, i.e.,

$$\int_0^{\infty} x\,dx\, J_0(xr)g_n(x,a) = w_n(r^2/4a^2) \tag{10}$$

for all positive r and

$$\int_0^\infty r\,dr\,J_0(xr)w_n(r^2/4a^2) = g_n(x,a) \tag{11}$$

for all positive x. If Eq. (8) is now Hankel transformed, naively supposing that it is legitimate to transform the right side termwise, there results

$$W^\infty(r;\omega)W_a(r) = \sum_{n=1}^\infty \frac{a_{2n}}{n}\,{}_2F_1\left(-n,n;\,1;\frac{r^2}{4a^2}\right) \tag{12}$$

[cf. Eq. (6)]. Equation (12) expresses the sought solution for the source coherence properties in terms of the expansion coefficients a_{2n}.

The legitimacy of Eq. (12) can be fully established, but involves rather a lot of classical analysis. I shall first formulate two key propositions that lead to Eq. (12).

Define the function $f(y)$ for $y\in[-1,1]$ by

$$f(y) = W^\infty\left[2a\left(\frac{1-y}{2}\right)^{1/2};\omega\right]W_a\left[2a\left(\frac{1-y}{2}\right)^{1/2}\right], \tag{13}$$

where a and ω are regarded as fixed.

Proposition 1: If $W^\infty(r;\omega)$ has a continuous second derivative for $0\leqslant r\leqslant 2a$, and if $I\subset(-1,1)$ is any closed interval, then there is a sequence $\{b_n\}$ of constants such that

$$f(y) = \sum_{n=1}^\infty b_n\,{}_2F_1\left(-n,n;\,1;\frac{1-y}{2}\right) \tag{14}$$

uniformly on I. This proposition can be proved by using the connection between ${}_2F_1(-n,n;1;x)$ and Legendre polynomials and by carefully using the theory of Legendre expansions. If in Eq. (14) one puts $y = 1-(r^2/2a^2)$, the proposition gives

$$W^\infty(r;\omega)W_a(r) = \sum_{n=1}^\infty b_n\,{}_2F_1\left(-n,n;\,1;\frac{r^2}{4a^2}\right) \tag{15}$$

uniformly on every closed interval $J\subset(0,2a)$. It is now a straightforward matter to deduce that

$$G_\omega(x,a) = 2\sum_{n=1}^\infty nb_n\,g_n(x,a) \tag{16}$$

for all positive x. (Actually, this follows if $x = z$, a general complex variable.)

Proposition 2: If

$$\sum_{n=1}^\infty C_n\frac{J_{2n}(2ax)}{x^2} = 0$$

for all positive x, then $C_n = 0$ for all $n = 1,2,\cdots$. This proposition shows that expansions of the form in Eqs. (8) and (16) have unique expansion coefficients, so that the identification $a_{2n} = nb_n$ follows.

An important additional fact about Eq. (12) emerges from the considerations of the previous paragraphs; namely, that the convergence in Eq. (12) is uniform on every closed interval contained in $(0,2a)$.

Proof of Proposition 1: First we note some properties of the first and second derivatives of $f(y)$, namely, that $f'(y)$ is continuous on $[-1,1)$, tending to infinity as y tends to 1, and $f''(y)$ is continuous on $(-1,1)$, tending to infinity as $y\to\pm 1$. Also note that $f(-1) = 0$ because $W_a(2a) = 0$.

Let I be any closed interval contained in $(-1,1)$. Since f is twice continuously differentiable on I, its Legendre expansion

$$f(y) = \sum_{k=0}^\infty \mu_k P_k(y)$$

(P_k denotes the standard Legendre polynomial) is uniformly convergent on I. Define the numbers b_n as follows:

$$\mu_0 = \tfrac{1}{2}b_1,\ \mu_1 = \tfrac{1}{2}(b_1+b_2),\ldots,\mu_k = \tfrac{1}{2}(b_k+b_{k+1}),\cdots.$$

It is easily verified that

$$\sum_{i=1}^{n+1} b_i\,{}_2F_1\left(-i,i;\,1;\frac{1-y}{2}\right) = \sum_{i=0}^{n}\mu_i P_i(y) + \tfrac{1}{2}b_{n+1}P_{n+1}(y),$$

because

$${}_2F_1(-n,n;\,1;\,x) = \tfrac{1}{2}[P_n(1-2x) + P_{n-1}(1-2x)],$$

which follows from the contiguity relations among hypergeometric functions.[4] Therefore

$$\left|f(y) - \sum_{i=1}^{n+1} b_i\,{}_2F_1\left(-i,i;\,1;\frac{1-y}{2}\right)\right| \leqslant \left|f(y) - \sum_{i=0}^{n}\mu_i P_i(y)\right| + \tfrac{1}{2}|b_{n+1}|\,|P_{n+1}(y)|.$$

For $y\in I$, we know that n can be taken large enough to make the first term on the right uniformly small. We will show that the same is true for the second term and thus establish the proposition.

First, we use the well-known bound

$$|P_{n+1}(y)| < \left(\frac{\pi}{2(n+1)(1-y^2)}\right)^{1/2},$$

which shows that there is a constant M such that

$$|P_{n+1}(y)| < M/(n+1)^{1/2} \tag{17}$$

for all $y\in I$. It is readily seen that

$$b_n = 2\mu_{n-1} - 2\mu_{n-2} + \cdots + (-1)^{n+1}2\mu_0.$$

Consequently,

$$|b_n| = 2|(\mu_0 - \mu_1 + \mu_2 - \cdots \pm \mu_{n-1})|,$$

which is the same as

$$|b_n| = 2\left|\sum_{k=0}^{n-1}\mu_k P_k(-1)\right|.$$

What we have is that

$$|b_{n+1}| = 2|s_n(-1)|,$$

where $s_n(-1)$ is the nth partial sum of the Legendre series for f evaluated at -1. By Christoffel's identity for Legendre polynomials,[5] we obtain

$$s_n(-1) = \frac{n+1}{2}\int_{-1}^1 f(t) \times\frac{(-1)^n P_{n+1}(t) - (-1)^{n+1}P_n(t)}{t+1}\,dt = (-1)^n\left(\frac{n+1}{2}\right)\int_{-1}^1\frac{f(t)}{t+1} \times[P_{n+1}(t) + P_n(t)]\,dt.$$

Therefore

$$|b_{n+1}| = (n+1)\left| \int_{-1}^{1} \phi(t) P_{n+1}(t)\, dt + \int_{-1}^{1} \phi(t) P_n(t)\, dt \right|, \tag{18}$$

where $\phi(t) = f(t)/(t+1)$. Let $p_n(x)$ denote the normalized Legendre polynomials, i.e.,

$$p_n(x) = \left(\frac{2n+1}{2}\right)^{1/2} P_n(x).$$

Equation (18) can now be expressed as

$$|b_{n+1}| = (n+1)\left| \left(\frac{2}{2n+3}\right)^{1/2} \int_{-1}^{1} \phi(t) p_{n+1}(t)\, dt + \left(\frac{2}{2n+1}\right)^{1/2} \int_{-1}^{1} \phi(t) p_n(t)\, dt \right|,$$

so that, using the inequality (17),

$$|b_{n+1}|\,|P_{n+1}(y)| < M(n+1)^{1/2}\left[\left(\frac{2}{2n+3}\right)^{1/2}\left| \int_{-1}^{1} \phi(t) p_{n+1}(t)\, dt \right| + \left(\frac{2}{2n+1}\right)^{1/2}\left| \int_{-1}^{1} \phi(t) p_n(t)\, dt \right|\right] \tag{19}$$

for all $y \in I$. Letting c_k denote the Legendre expansion coefficients of the function ϕ, the inequality (19) can be written as

$$|b_{n+1}|\,|P_{n+1}(y)| < M\left[\left(\frac{n+1}{n+\frac{3}{2}}\right)^{1/2}|c_{n+1}| + \left(\frac{n+1}{n+\frac{1}{2}}\right)^{1/2}|c_n|\right]. \tag{20}$$

With the inequality (20), the proof is almost complete. It is known that the Legendre expansion coefficients of a square-integrable function on $[-1,1]$ tend to zero with increasing order. Since ϕ is such a function, $|c_n| \to 0$ as $n \to \infty$, so that the left side of (20) can be made uniformly small on I by taking n large enough. This completes the proof.

Proof of Proposition 2: First we show that $C_1 = 0$. The approach is to prove that the series in question, namely,

$$\sum_{n=1}^{\infty} C_n \frac{J_{2n}(y)}{y^2} = 0,$$

converges uniformly for y (0,1], so that

$$\lim_{y \to 0} \sum_{n=1}^{\infty} C_n \frac{J_{2n}(y)}{y^2} = \sum_{n=1}^{\infty} C_n \lim_{y \to 0} \frac{J_{2n}(y)}{y^2},$$

which allows us to conclude that $C_1 = 0$.

Clearly,

$$\sum_{n=1}^{\infty} C_n J_{2n}(y) = 0$$

for all $y > 0$. Since the sum on the left is a Neumann series, it follows from Pincherle's theorem[6] that

$$\sum_{n=1}^{\infty} C_n J_{2n}(z)$$

converges for all complex z and that the associated power series

$$\sum_{n=1}^{\infty} \frac{C_n}{2^{2n}(2n)!} z^{2n}$$

also has an infinite radius of convergence. Consequently,

$$\sum_{n=1}^{\infty} \frac{|C_n|}{2^{2n}(2n)!}$$

converges because of the absolute convergence of power series. We also have that

$$|J_{2n}(z)| \leqslant \frac{|z|^{2n}}{2^{2n}(2n)!}$$

for all complex z, so that

$$\left| C_n \frac{J_{2n}(y)}{y^{2k}} \right| \leqslant |C_n| \frac{y^{2n-2k}}{2^{2n}(2n)!} \tag{21}$$

for all positive y and all $k = 1,2,3,\cdots$. In particular, if $k = 1$ and $y \leqslant 1$,

$$\left| C_n \frac{J_{2n}(y)}{y^2} \right| \leqslant |C_n| \frac{1}{2^{2n}(2n)!},$$

which shows by Weierstrass' test that

$$\sum_{n=1}^{\infty} C_n \frac{J_{2n}(y)}{y^2}$$

converges uniformly to zero on (0,1]. Hence, $C_1 = 0$.

We complete the proof using mathematical induction. Suppose we have shown that $C_1 = C_2 = \cdots = C_N = 0$. Then

$$\sum_{n=N+1}^{\infty} C_n \frac{J_{2n}(y)}{y^2} = 0$$

for all positive y. Clearly then,

$$\sum_{n=N+1}^{\infty} C_n \frac{J_{2n}(y)}{y^{2(N+1)}} = 0 \tag{22}$$

also for all $y > 0$. Putting $k = N+1$ in Eq. (21), we get

$$\left| C_n \frac{J_{2n}(y)}{y^{2(N+1)}} \right| \leqslant |C_n| \frac{2^{2n-2(N+1)}}{2^{2n}(2n)!},$$

which for $n \geqslant N+1$ and $y \leqslant 1$ implies

$$\left| C_n \frac{J_{2n}(y)}{y^{2(N+1)}} \right| \leqslant |C_n| \frac{1}{2^{2n}(2n)!}.$$

It follows that the series in Eq. (22) is uniformly convergent on (0,1], and this shows that $C_{N+1} = 0$. Hence, the proposition follows by induction.

I close with several remarks about the solution presented. First, it is in fact possible to determine the expansion coefficients in Eq. (8) from a knowledge of the far-field intensity pattern alone. One only needs to exploit the relationship between the Maclaurin expansion coefficients of $G_\omega(z,a)$ and those of Eq. (8).[7] Second, the result

$${}_2F_1(-n,n;1;x) = \tfrac{1}{2}[P_n(1-2x) + P_{n-1}(1-2x)] \tag{23}$$

shows that the hypergeometric functions needed for the solution not only are finite polynomials, but have a simple expression in terms of well-studied orthogonal polynomials. Finally, the interesting question of the stability of the solution with respect to small perturbations in the intensity pat-

tern should be raised. The possibility of deducing the coherence properties of a source from careful measurements of its far-field intensity pattern would require such stability.

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Quantum statistics of multimode m-photon absorption process [a)]

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A density matrix method is used to obtain an exact solution for the reduced density matrix of the field in an arbitrary multimode m-photon absorption process. The results of some earlier specialized studies of photon statistics in multiphoton absorption process can be recovered from this solution.

It is well known that nonlinear interaction of light with matter changes the quantum statistical properties of the light field.[1] The changes of the photon statistics depend on the interaction process and on the initial conditions of the field.

In this paper we consider a multimode m-photon absorption process. The multiphoton absorption processes have recieved a great deal of attention in recent years due to the possibility of producing a radiation field which shows photon antibunching. The photon statistics of two-photon absorption process was studied using a generating function approach and exact expressions for the photon distribution function were given in single-mode[2-5] and two-mode[6] processes. The off-diagonal elements of the density matrix of the field in the single- and two-mode two-photon absorption processes were given by Simaan and Loudon.[7,8] Paul, Mohr, and Brunner[9] studied the photon statistics of m-photon absorption process on the basis of an approximate procedure. Recently, an exact analytic solution of the master equation describing single-mode m-photon absorption has been obtained by Zubairy and Yeh[10] using a density matrix approach and by Voigt, Bandilla, and Ritze[11] using a Laplace transform method.

In the present paper we extend these results to arbitrary multimode absorption process. We begin by considering the master equation which describes a multimode m-photon process. We present the exact solution of the reduced density matrix of the field using the matrix approach.[10] Due to the general nature of our problem the results of the earlier studies can be recovered in the appropriate limits.

We consider a coupled system of a field and N noninteracting two-level atoms in their ground state. The number of atoms N in the lower level are assumed to be maintained constant by some external influence. We assume that the atoms make a transition from the lower level to the upper level by absorbing m photons; x_i photons in mode i ($i = 1, 2, ..., l$; $l \leqslant m$). We then obtain

$$\sum_{i=1}^{l} x_i = m. \tag{1}$$

The single-mode situation corresponds to the case when one of the x_i's such as x_1 is equal to m and all the rest are zero. The reduced density matrix $\hat{\rho}_F$ of the field can then be shown to satisfy the following equation of motion using the standard perturbation techniques

$$\frac{d\hat{\rho}_F}{dt} = -\beta^{(m)}\left[\left(\prod_{i=1}^{l}\hat{a}_i^{\dagger x_i}\right)\left(\prod_{i=1}^{l}\hat{a}_i^{x_i}\right)\hat{\rho}_F - 2\left(\prod_{i=1}^{l}\hat{a}_i^{x_i}\right)\hat{\rho}_F \times\left(\prod_{i=1}^{l}\hat{a}_i^{\dagger x_i}\right) + \hat{\rho}_F\left(\prod_{i=1}^{l}\hat{a}_i^{\dagger x_i}\right)\left(\prod_{i=1}^{l}\hat{a}_i^{x_i}\right)\right], \tag{2}$$

where $\beta^{(m)}$ is the absorption coefficient for m-photon absorption, and $\hat{a}_i^{\dagger}$, $\hat{a}_i$ are the photon creation and destruction operators of the ith mode, respectively. In Eq. (2) the saturation of the absorbing atoms is neglected.

We denote the state in which there are n_i photons in the ith mode ($i = 1, 2, ..., l$) by $|n_1, n_2 ... n_l\rangle$. The equation of motion (2) for $\hat{\rho}_F$ can be translated into an equation for the matrix element

$$\rho(n_1, ..., n_l; n_1 + K_1, ..., n_l + K_l, \tau) = \langle n_1, ..., n_l|\hat{\rho}_F|n_1 + K_1, ..., n_l + K_l\rangle, \tag{3}$$

of the reduced density matrix by evaluating the matrix element of each term in Eq. (2) between the appropriate Fock states. The resulting equation is

$$\frac{\partial\rho(n_1, ..., n_l; n_1 + K_1, ..., n_l + K_l;\tau)}{\partial\tau} = a(n_1, ..., n_l; n_1 + K_1, ..., n_l + K_l)\rho(n_1, ..., n_l; n_1 + K_1, ..., n_l + K_l; \tau) + b(n_1 + x_1, ..., n_l + x_l; n_1 + x_1 + K_1, ..., n_l + x_l + K_l) \times\rho(n_1 + x_1, ..., n_l + x_l; n_1 + x_1 + K_1, ..., n_l + x_l + K_l; \tau), \tag{4}$$

where $\tau = 2\beta^{(m)}t$ and

$$a(n_1, ..., n_l; n_1', ..., n_l') = -\frac{1}{2}\left[\prod_{j=1}^{l}\frac{n_j!}{(n_j - x_j)!} + \prod_{j=1}^{l}\frac{n_j'!}{(n_j' - x_j)!}\right], \tag{5a}$$

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$$b(n_1, ..., n_l; n_1', ..., n_l') = \left[\prod_{j=1}^{l} \frac{n_j! n_j'!}{(n_j - x_j)!(n_j' - x_j)!}\right]^{1/2}. \tag{5b}$$

Following the method employed in Ref. 10, we first express Eq. (4) in the matrix notation

$$\frac{\partial}{\partial \tau} \rho_{i_1,...,i_l}(\tau) = M_{i_1,...,i_l} \rho_{i_1,...,i_l}(\tau), \tag{6}$$

where

$$\rho_{i_1,...,i_l}(\tau) = \begin{bmatrix} \rho(i_1, ..., i_l;\ i_1 + K_1, ..., i_l + K_l;\ \tau) \\ \rho(i_1 + x_1, ..., i_l + x_l;\ i_1 + K_1 + x_1, ..., i_l + K_l + x_l;\ \tau) \\ \vdots \\ \rho(i_1 + nx_1, ..., i_l + nx_l;\ i_1 + K_1 + nx_1, ... i_l + K_l + nx_\rho;\ \tau) \\ \vdots \end{bmatrix}, \tag{7}$$

$$M_{i_1,...,i_l} = \begin{bmatrix} m_{00} & m_{01} & & & \\ & m_{11} & m_{12} & & \\ & & \ddots & & \\ & & & m_{nn} & m_{n\,n+1} \end{bmatrix}. \tag{8}$$

In Eq. (8), the elements m_{jk} are given by the following expressions

$$m_{jj} = a(i_1 + jx_1, ..., i_l + jx_l;\ i_1 + K_1 + jx_1, ..., i_l + K_l + jx_l), \tag{9a}$$

$$m_{j\,j+1} = b(i_1 + (j+1)x_1, ..., i_l + (j+1)x_l;\ i_1 + K_1 + (j+1)x_1, ..., i_l + K_l + (j+1)x_l), \tag{9b}$$

for $j = 0, 1, 2, \cdots$.

The solution of Eq. (6) or Eq. (4) can be expressed in the form

$$\rho(i_1 + nx_1, ..., i_l + nx_l;\ i_1 + K_1 + nx_1, ..., i_l + K_l + nx_l; \tau) = \sum_{s=0}^{\infty} \sum_{q=0}^{\infty} \alpha_n^{s;i_1,...,i_l} \beta_q^{s;i_1,...,i_l} e^{\lambda_{s;i_1,...,i_l}\tau} \rho(i_1 + qx_1, ..., i_l + qx_l; \times i_1 + K_1 + qx_1, ..., i_l + K_l + qx_l;\ 0), \tag{10}$$

where $\lambda_{s;i_1,...,i_l}$ are the eigenvalues of the matrix $M_{i_1,...,i_l}$, i.e., they satisfy the equation,

$$\det[M_{i_1,...,i_l} - \lambda I] = 0, \tag{11}$$

(I being the unit matrix), $\alpha_n^{s;i_1,...,i_l}$ is the nth element of the right eigenstate of $M_{i_1,...,i_l}$ corresponding to the eigenvalue $\lambda_{s;i_1,...,i_l}$, and $\beta_q^{s;i_1,...,i_l}$ is the qth element of the left eigenstate of $M_{i_1,...,i_l}$ corresponding to the eigenvalue $\lambda_{s;i_1,...,i_l}$. The matrix elements $\alpha_n^{s;i_1,...,i_l}$ and $\beta_q^{s;i_1,...,i_l}$ can be shown to obey the following recursion relations

$$m_{n-1\,n-1}\alpha_{n-1}^{s;i_1,...,i_l} + m_{n-1\,n}\alpha_n^{s;i_1,...,i_l} = m_{ll}\alpha_{n-1}^{s;i_1,...,i_l}, \tag{12a}$$

$$m_{q-1\,q}\beta_{q-1}^{s;i_1,...,i_l} + m_{qq}\beta_q^{s;i_1,...,i_l} = m_{ll}\beta_q^{s;i_1,...,i_l}. \tag{12b}$$

By solving Eq. (11) and by iterating the recursion relations (12a) and (12b), we obtain

$$\lambda_{s;i_1,...,i_l} = m_{ss}, \tag{13}$$

$$\alpha_n^{s;i_1,...,i_l} = \begin{cases} \prod_{r=n+1}^{s} \left(\frac{m_{r-1\,r}}{m_{ss} - m_{r-1\,r-1}}\right); & n \leqslant s, \\ 0; & n > s, \end{cases} \tag{14}$$

$$\beta_q^{s;i_1,...,i_l} = \begin{cases} \prod_{r=s+1}^{q} \left(\frac{m_{r-1\,r}}{m_{ss} - m_{rr}}\right); & q \geqslant s, \\ 0; & q < s. \end{cases} \tag{15}$$

If we let $n = 0$, $i_j = n_j$, and $K_j = n_j' - n_j$ ($j = 1, 2 ... l$) in Eq. (10), then, on substituting from Eqs. (9a), (9b), and (13)–(15), it follows

$$\rho(n_1, ..., n_l; n_1', ...n_l';\ \tau) = \sum_{s=0}^{\infty} \sum_{q=s}^{\infty} \frac{\Pi_{r=1}^{q} b(n_1 + rx_1, ..., n_l + rx_l; n_1' + rx_1, ..., n_l' + rx_l)}{\Pi_{\substack{r=0 \\ r \neq s}}^{q} [a(n_1 + sx_1, ..., n_l + sx_l; n_1' + sx_1, ..., n_l' + sx_l) - a(n_1 + rx_1, ..., n_l + rx_l;\ n_1' + rx_1, ..., n_l' + rx_l)]} \times e^{a(n_1 + sx_1, ..., n_l + sx_l; n_1' + sx_1, ..., n_l' + sx_l)\tau} \rho(n_1 + qx_1, ..., n_l + qx_l; n_1' + qx_1, ...n_l' + qx_l, 0). \tag{16}$$

This equation, combined with the expressions for a's and b's [cf. Eqs. (5a) and (5b)], completely determines the time evolution of the density matrix. The photon distribution function $p(n_1, ..., n_l;\ \tau) = \langle n_1, ..., n_l | \hat{\rho}_F | n_1, ..., n_l \rangle$ can be determined from Eq. (16) by putting $n_j' = n_j$ ($j = 1, ..., l$).

We now show how some of the earlier specialized results regarding multiphoton absorption processes can be obtained from Eq. (16).

In the case of single-mode m-photon absorption process, one of the x_i's (say x_1) is equal to m and all the rest are

zero. We then obtain, from Eqs. (5a) and (5b), that

$$a(n_1;\ n_1') = -\frac{1}{2}\left(\frac{n_1!}{(n_1-m)!} + \frac{n_1'!}{(n_1'-m)!}\right), \tag{17a}$$

$$b(n_1;\ n_1') = \left(\frac{n_1!n_1'!}{(n_1-m)!(n_1'-m)!}\right)^{1/2}. \tag{17b}$$

If follows from Eq. (16) that

$$\rho(n_1;\ n_1';\ \tau) = \sum_{s=0}^{\infty}\sum_{q=s}^{\infty} \frac{\Pi_{r=1}^{q} b(n_1+mr;\ n_1'+mr)}{\Pi_{\substack{r=0\\ r\neq s}}^{q}\left[a(n_1+ms;\ n_1'+ms) - a(n_1+mr;\ n_1'+mr)\right]} e^{a(n_1+ms;n_1'+ms)\tau}\rho(n_1+mq;\ n_1'+mq;\ 0). \tag{18}$$

After making some rearrangements, this equation can be shown to be identical to Eq. (31) in Ref. 10 (see also Ref. 11 for the case $n_1 = n_1'$). We have discussed some aspects of photon statistics in single-mode m-photon abosorption process, such as photon antibunching, in that paper.

As another example, we consider m-mode m-photon absorption process. In this case, $l = m$ and $x_i = 1 (i = 1, 2, ..., m)$. The expressions for a and b in Eqs. (5a) and (5b) then become

$$a(n_1, ..., n_m;\ n_1', ..., n_m') = -\tfrac{1}{2}[n_1..., n_m + n_1' ..., n_m'], \tag{19a}$$

$$b(n_1, ..., n_m;\ n_1', ..., n_m') = (n_1 ..., n_m n_1' ..., n_m')^{1/2}. \tag{19b}$$

Moreover, from Eq. (16), we obtain the following solution for the density matrix

$$\rho(n_1, ..., n_m;\ n_1', ..., n_m';\ \tau) = \sum_{s=0}^{\infty}\sum_{q=s}^{\infty} \frac{\Pi_{r=1}^{q} b(n_1+r, ..., n_m+r;\ n_1'+r, ...n_m+r)}{\Pi_{\substack{r=0\\ r\neq s}}^{q}\left[a(n_1+s_1, ..., n_m+s;\ n_1'+s, ..., n_m'+s) - a(n_1+r, ..., n_m+r;\ n_1'+r, ..., n_m'+r\right]}$$

$$\times e^{a(n_1+s,...,n_m+s;n_1'+s,...,n_m'+s)\tau}\rho(n_1+q, ..., n_m+q;\ n_1'+q, ..., n_m'+q;\ 0). \tag{20}$$

Simaan and Loudon[6,8] have discussed the case $m = 2$ in some detail. Equation (20) together with Eqs. (19a) and (19b), after some rearrangement, can be shown to reduce to their results. For a discussion of the quantum statistical properties of the double-beam two-photon absorption process, we refer the reader to Ref. 6.

In conclusion, we have obtained an exact solution of the master equation that describes an arbitrary multimode multiphoton process. We have shown via two examples how the results of the earlier specialized studies can be recovered from this general solution.

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