Explicit expressions for double Gel'fand states

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Double Gel'fand states are given explicitly as polynomials of boson operators. The coefficients of these polynomials may be expressed in terms of recoupling coefficients of external products of permutation groups or Kronecker products within the unitary group, as well as in terms of multiple Clebsch–Gordan coefficients of the unitary group.

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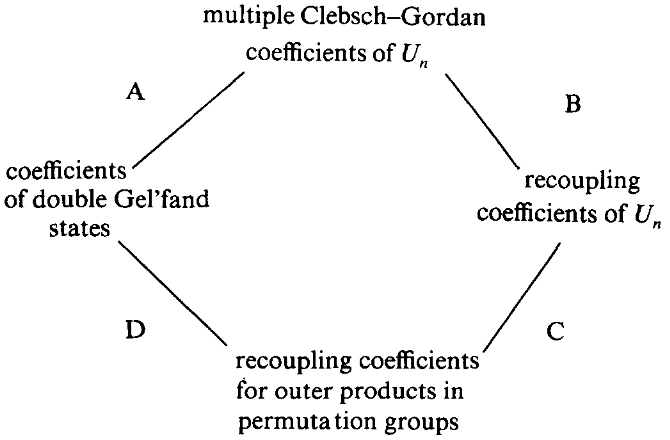
I. INTRODUCTION

Double Gel'fand states emerge naturally from the treatment of representations of the unitary group in terms of boson polynomials (see Louck[1] and references therein). They prove to be a powerful tool (Chacón *et al.*[2] and Louck and Biedenharn[3]) in this context, but they are also useful in establishing connections to the permutation group.[4–6] Furthermore, they may be used explicitly to describe physical systems.[7]

A close study of the explicit expressions for these states is justified as they are basic for many applications[5,7]. One such expression was given by Louck and Biedenharn,[3] and a different one in Refs. 5 and 6.

In the present paper we shall give three closed expressions: A first one in terms of multiple Clebsch–Gordan coefficients of U_n. This expression may be shown to be closely related to the one given by Louck and Biedenharn.[3] Next we proceed to obtain an expression in terms of recoupling coefficients for the Kronecker product in U_n. Finally we shall show that this expression may be reinterpreted in terms of certain recoupling coefficients for external products of permutation groups. This expression is identical to the one obtained in Ref. 5, if a mistake in the normalization given there is corrected (see Appendix).

The following diagram illustrates the relations for the coefficients of each monomial if a double Gel'fand state is given as a boson polynomial.



In the next section we shall give some preliminaries concerning double Gel'fand states and fix the notation we shall use. Then we proceed to prove the steps A, B, and C, as indicated in the diagram. The proof of step A will be very different from the derivation of a similar result given by Louck and Biedenharn[3] and will only use standard vector coupling techniques. Step B will be proved in a quite elementary way, generalizing a method used in Ref. 8. To prove step C, we shall employ the concept of special Gel'fand states,[4] generalizing a technique developed previously for special cases.[9] The above diagram could be completed by the proof of D as given in Ref. 5 but we shall not reproduce this proof, as it is given in the reference, and its methods differ basically from the ones used in this paper. We shall only discuss in an appendix how the normalization constant, as presented in Ref. 5, must be corrected, to coincide with our result from step C.

Many of the results of this paper are known at least for special cases. Nevertheless, we believe that this presentation is relevant not only because it gives the results in full generality but especially because all results are obtained by standard techniques and do not require the introduction of new complicated concepts as the proofs in Louck and Biedenharn[3] and Ref. 5 .The only exception is the use of special Gel'fand states, but these are only relevant to establish the connection with S_N.

Most of the content of this paper is contained in a thesis by one of us.[10]

II. DOUBLE GEL'FAND STATES AS BOSON POLYNOMIALS

Two standard representations for double Gel'fand states are used in the literature; one[1,3] in terms of creation operators for harmonic oscillator wavefunctions (boson operators), the other[5] in terms of the variables of a complex Bargmann space.[11] The two formulations are equivalent, and we shall here adopt the former.

We thus formally consider an harmonic oscillator in n^2 dimensions. Denoting coordinates and momenta by x_j^s, p_j^s $(s,j = 1,...,n)$, we may define the creation operators $\eta_j^s = (1/\sqrt{2})(x_j^s - ip_j^s)$ and the annihilation operators $\xi_j^s = (\eta_j^s)^\dagger$, where $\dagger$ denotes Hermitian conjugation. Clearly we have

$$[\eta_i^s, \xi_j^t] = \delta_{st}\delta_{ij}, \quad [\eta_i^s, \eta_j^t] = [\xi_i^s, \xi_j^t] = 0.$$

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The operators

$$\mathbb{C}^{st}_{ij} = \eta^s_i \xi^t_j \tag{2.1}$$

now form a Lie Algebra for $\mathbb{U}_{n^2}$ under commutation [,]. This algebra, defined as an operator algebra over polynomials of η (boson polynomials), only admits the completely symmetric representations $[N0\cdots0]$, spanned by the set of all monomials of degree N. By contraction we can form two Lie algebras with generators

$$\mathscr{C}^{st} = \sum_j \mathbb{C}^{st}_{jj} \tag{2.2a}$$

and

$$C_{ij} = \sum_s \mathbb{C}^{ss}_{ij} \tag{2.2b}$$

that generate two unitary groups in n dimensions denoted by $\mathscr{U}_n$ and U_n that refer to the upper and lower labels respectively. Clearly their direct product is a subgroup $U_n \times \mathscr{U}_n \subset \mathbb{U}_{n^2}$.

It is well known[1] that the irreducible representations (IR's) of U_n and $\mathscr{U}_n$ must be equivalent to be contained in $[N0\cdots0]$ and thus to be realized on the space of the boson polynomials. These IR's are characterized by a partition of N into a sum of n positive integers.

If a polynomial transforms according to an IR of one of the groups U_n or $\mathscr{U}_n$, then it transforms according to the same IR of the other one. The row labels with respect to the two groups are independent and we have a d^2_α-dimensional vector space, all of whose members transform according to an IR α of dimensions d_α with respect to either group.

We choose the row labels for both groups as Gel'fand schemes, that is, by characterizing them through the IR of the chain of subgroups

$$\mathscr{U}_n \supset \mathscr{U}_{n-1} \supset \cdots \supset \mathscr{U}_2 \supset \mathscr{U}_1,$$

and similarly for U_n. These IR's are successively partitions of positive integers ($\leqslant N$) into n, $n-1$, $n-2$, etc., positive integers and may be arranged into triangular patterns that characterize the row label of an IR $[g] \equiv [g^n_1, g^n_2, \ldots, g^n_n]$. Such a pattern, called a Gel'fand scheme, is denoted by

$$\backslash g/ = \begin{matrix} g^{n-1}_1 & & \cdots & & g^{n-1}_{n-1} \\ & g^{n-2}_1 & \cdots & g^{n-2}_{n-2} & \\ & \ddots & & \iddots & \\ & & g^1_1 & & \end{matrix} \tag{2.3}$$

The number g^i_j must fulfill the "betweeness" conditions

$$g^i_j \geqslant g^{i-1}_j \geqslant g^i_{j+1}. \tag{2.4}$$

A further important concept is that of the weight of a Gel'fand pattern defined by

$$w_s = \sum_{j=1}^{s} g^s_j - \sum_{j=1}^{s-1} g^{s-1}_j.$$

If $[g]$ is a partition of the type $[m0\cdots0] \equiv m$, then the vector $\mathbf{w}$ formed of all weights characterizes the pattern uniquely, and we shall often use the labels m and $\mathbf{w}$ instead of $[g]$ and $\backslash g/$ to denote such situations. If, in turn, the weight vector has only one component different from zero, $[g]$ must be of the type $[m0\cdots0]$ and the nonzero component of $\mathbf{w}$ must equal m. We shall then denote $[g]$ and $\backslash g/$ by m and i, where i indicates the component of $\mathbf{w}$ that is unequal to zero.

To be quite clear, the above notation implies that a basis vector of U_n usually given by the pattern

$$\begin{matrix} g^n_1 & & \cdots & & g^n_n \\ & g^{n-1}_1 & \cdots & g^{n-1}_{n-1} & \\ & \ddots & & \iddots & \\ & & g^1_1 & & \end{matrix} \equiv \begin{matrix}[g]\\ \backslash g/\end{matrix} \equiv [g];\backslash g/, \tag{2.5}$$

will now be denoted for the special cases mentioned above as

$$\begin{matrix} m\ 0 & & \cdots & & 0 \\ & \left(\sum_{i=1}^{n-1} w_i\right)0 & \cdots & 0 & \\ & \ddots & & \iddots & \\ & & (w_1+w_2)0 & & \\ & & w_1 & & \end{matrix} \equiv \begin{matrix} m \\ \mathbf{w} \end{matrix} \equiv m;\mathbf{w}, \tag{2.6}$$

$$\begin{matrix} m\ 0 & & \cdots & & 0 \\ & m\ 0 & \cdots & 0 & \\ & \ddots & & \iddots & \\ & & m\ 0 \ \cdots \ 0 & & \\ i-1\ \text{rows} \left\{ \right. & & \begin{matrix} 0 & \cdots & 0 \\ & \ddots\ \iddots & \\ & 0 & \end{matrix} & & \end{matrix} \equiv \begin{matrix} m \\ i \end{matrix} \equiv m;i. \tag{2.7}$$

We shall use notations with the row labels below or next to the representation label according to typographic convenience. When considering double Gel'fand states, we introduce similar notation for $\mathscr{U}_n$ and U_n, i.e., for upper and lower labels; preferably we shall use the letter h when referring to the lower and the letter g when referring to the upper indices, and we shall usually put the row labels in the corresponding upper or lower position.

As mentioned above, we must have equal partitions for the IR's of U_n and $\mathscr{U}_n$ and thus we have $h^n_i = g^n_i \equiv f_i$, $1 \leqslant i \leqslant n$, where we introduce the last notation, f_i to avoid asymmetry. A double Gel'fand state now is written as

$$\left\langle \eta_{i;}^{s;}\begin{matrix} s=1,\dots,n \\ i=1,\dots,n\end{matrix} \middle| \begin{matrix} /g\backslash \\ [f] \\ \backslash h / \end{matrix} \right\rangle \tag{2.8}$$

where / \ indicates an inverted Gel'fand scheme, and the bra indicates a representation as a boson polynomial. In a double Gel'fand state we have a second set of weights

$$\overline{w}_i = \sum_{j=1}^{i} h_j^i - \sum_{j=1}^{i-1} h_j^{i-1}.$$

The first weight w is associated with the upper, the second $\overline{\mathbf{w}}$ with the lower labels. A pattern is said to be of highest weight if $w_i = f_i$ for all $1 < i < n$, and similarly we have a double state of highest weight if both patterns are of highest weight. The weight w_s is the eigenvalue of $\mathscr{C}^{ss}$ and is thus equal to the sum over i of the exponents of η_i^s in a state. This sum must be constant for all terms of the polynomial that forms the state. A similar argument applies to $\overline{w}_i$ for the lower labels [cf. Eqs. (2.10a) and (2.10b)].

Double Gel'fand states of highest weight are proportional to products of determinants of boson operators[1] and are thus readily available. All other double Gel'fand states may in principle be obtained by applying lowering operators[12] to the polynomials, first to the upper, then to the lower indices. The result must be a homogeneous polynomial in the η_i^s and may be written as

$$\left\langle \eta_{i;}^{s;}\begin{matrix} s=1,\dots,n \\ i=1,\dots,n\end{matrix} \middle| \begin{matrix} /g\backslash \\ [f] \\ \backslash h / \end{matrix} \right\rangle = \sum_{\mathsf{D}} \mathsf{C}(\mathsf{D};[f],\backslash g/,\backslash h/) \prod_{i,s=1}^{n} \frac{(\eta_i^s)^{D_{si}}}{(D_{si}!)^{1/2}}, \tag{2.9}$$

where D is a $n \times n$ matrix with elements D_{si} that fulfill

$$\sum_i D_{si} = w_s, \tag{2.10a}$$

$$\sum_s D_{si} = \overline{w}_i. \tag{2.10b}$$

The last equations express a property of the weights mentioned above. The factor $1/(D_{si}!)^{1/2}$ was introduced for convenience, since then each monomial is a normalized oscillator function.

Various explicit expressions for coefficients **C** will be derived in the following sections.

III. EXPRESSIONS IN TERMS OF MULTIPLE CLEBSCH-GORDAN COEFFICIENTS

In order to express double Gel'fand states in terms of multiple Clebsch–Gordan coefficients, we use the fact that the basic building block of the expression (2.9) is $(\eta_i^s)^{D_{si}}/(D_{si}!)^{1/2}$; this simple monomial clearly transforms according to an IR $[D_{si}0\cdots0]$ of U_n and $\mathscr{U}_n$. The corresponding double Gel'fand state is characterized uniquely by the weights $w''_\tau = \delta_{\tau s} D_{si}, \overline{w}''_j = \delta_{ji} D_{si}$.

Next we may consider a monomial of the form $\Pi_i(\eta_i^s)^{D_{si}}/(D_{si}!)^{1/2}$. Such a product transforms according to the IR $w_s = [w_s 0\cdots0]$ [w_s given by Eq. (2.10a)]. Again the weight determines the state completely. For the upper indices we have $w'_\tau = \delta_{s\tau} w_s$, and for the lower ones $\overline{\mathbf{w}}' = \mathbf{D}_s = [D_{s1} D_{s2} \cdots D_{sn}]$.

Considering notation established in (2.6) and (2.7), we may write

$$\left\langle \eta_{i;}^{s;}\begin{matrix} s \text{ fixed} \\ i=1,\dots,n\end{matrix} \middle| w_s; \begin{matrix} s \\ \mathbf{D}_s \end{matrix} \right\rangle = \prod_{i=1}^{n} \frac{\eta_i^{s\,D_{si}}}{(D_{si}!)^{1/2}}. \tag{3.1}$$

Here the s refers to $\mathscr{U}_n$ and the $\mathbf{D}_s$ to the U_n row labels. For reasons that will become apparent later, we now proceed to couple two such states to one transforming according to the IR $[g^2] \equiv [g_1^2 g_2^2 0\cdots0]$. We perform this coupling using Clebsch–Gordan coefficients of U_n and summing over different possible values of $\mathbf{D}_1$ and $\mathbf{D}_2$. To choose the lower pattern for the coupling is essential, because all possible row labels of w_s are of the type required, whereas the upper labels are fixed.

We thus write

$$\left\langle \eta_{i;}^{s;}\begin{matrix} s=1,2 \\ i=1,\dots,n\end{matrix} \middle| \begin{matrix} /g^2\backslash \\ [g^2] \\ \backslash \gamma^2 / \end{matrix} \right\rangle = \sum_{\mathbf{D}_1,\mathbf{D}_2} \left\langle \eta_{i;}^{s;}\begin{matrix} s=1 \\ i=1,\dots,n\end{matrix} \middle| w_1; \begin{matrix} 1 \\ \mathbf{D}_1 \end{matrix} \right\rangle \left\langle \eta_{i;}^{s;}\begin{matrix} s=2 \\ i=1,\dots,n\end{matrix} \middle| w_2; \begin{matrix} 2 \\ \mathbf{D}_2 \end{matrix} \right\rangle \left\langle \begin{matrix} w_1 & w_2 \\ \mathbf{D}_1 & \mathbf{D}_2 \end{matrix} \middle| \begin{matrix} g_1^2 g_2^2 0\cdots0 \\ \backslash \gamma^2 / \end{matrix} \right\rangle, \tag{3.2}$$

where the last coefficient on the right is a Clebsch–Gordan coefficient. Here $\backslash \gamma^2 /$ is any pattern compatible with the IR $[g_1^2 g_2^2 0\cdots0]$, and we define

$$/g^i\backslash \equiv \begin{array}{ccccccc} & & & g_1^1 & & & \\ & & g_1^2 & & g_2^2 & & \\ & \cdot^{\cdot^{\cdot}} & & & & \ddots & \\ & g_1^i & g_2^i & \cdots & & g_i^i & \\ \cdot^{\cdot^{\cdot}} & & & \cdot^{\cdot^{\cdot}} & & & 0 \\ g_1^i & g_2^i & \cdots & g_i^i & 0 & \cdots & 0 \end{array} \tag{3.3}$$

The upper pattern then has to be $/g^2$ because $g_1^1 = w_1$ and all weights for $s > 2$ are zero. It is now clear that we intend to proceed by successive coupling, using the recursive formula

$$\left\langle \eta_i^s;\begin{matrix} s=1,\dots,t+1\\ i=1,\dots,n\end{matrix}\middle| \begin{matrix}/g^{t+1}\backslash\\ [g^{t+1}]\\ \backslash\gamma^{t+1}/\end{matrix}\right\rangle = \sum_{\backslash\gamma^t/,\mathbf{D}_{t+1}} \left\langle \eta_i^s; \begin{matrix} s=1,\dots,t\\ i=1,\dots,n\end{matrix}\middle|\begin{matrix}/g^t\backslash\\ [g^t]\\ \backslash\gamma^t/\end{matrix}\right\rangle \left\langle \eta_i^s;\begin{matrix}s=t+1\\ i=1,\dots,n\end{matrix}\middle| w_{t+1}; \begin{matrix} t+1\\ \mathbf{D}_{t+1}\end{matrix}\right\rangle \left\langle \begin{matrix}[g^t] & w_{t+1}\\ \backslash\gamma^t/ & \mathbf{D}_{t+1}\end{matrix}\middle|\begin{matrix}[g^{t+1}]\\ \backslash\gamma^{t+1}/\end{matrix}\right\rangle. \tag{3.4}$$

Again the upper pattern is completely fixed as we add weight only in one row that previously had weight zero. Here and in what follows we use any partition with i numbers different from zero to identify an IR of any group U_j, $i\leqslant j\leqslant n$ without adding or dropping the zeros in question explicitly.

Note that the Clebsch-Gordan coefficients involved are free of multiplicities since one of the partitions is always of the one row type. Explicit expressions for these coefficients are given by Chacón *et al.*[2]

We now choose the patterns $\backslash\gamma^n/\equiv\backslash\, h\,/$ and $/\,g\backslash\equiv/\,g^n\backslash$. Applying (3.4) repeatedly, we obtain

$$\begin{aligned}\left\langle \eta_i^s;\begin{matrix} s=1,\dots,n\\ i=1,\dots,n\end{matrix}\middle| \begin{matrix}/\,g\backslash\\ [f]\\ \backslash\, h\,/\end{matrix}\right\rangle &= \sum_{\mathbf{D}_1,\mathbf{D}_2,\dots,\mathbf{D}_n} \left\langle \left[\left[\left[\begin{matrix} w_1 w_2\\ \mathbf{D}_1\mathbf{D}_2\end{matrix}\right]\begin{matrix}[g^2]w_3\\ \mathbf{D}_3\end{matrix}\right]\cdots\right]\begin{matrix}[g^{n-1}]w_n\\ \mathbf{D}_n\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle \prod_{s=1}^{n}\left\langle \eta_i^s;\begin{matrix} s\text{ fixed}\\ i=1,\dots,n\end{matrix}\middle| w_s;\begin{matrix} s\\ \mathbf{D}_s\end{matrix}\right\rangle\\ &= \sum_{\mathsf{D}}\left\langle \left[\left[\left[\begin{matrix} w_1 w_2\\ \mathbf{D}_1\mathbf{D}_2\end{matrix}\right]\begin{matrix}[g^2]w_3\\ \mathbf{D}_3\end{matrix}\right]\cdots\right]\begin{matrix}[g^{n-1}]w_n\\ \mathbf{D}_n\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle \prod_{s,i=1}^{n}\frac{\eta_i^{sD_{si}}}{\sqrt{D_{si}!}},\end{aligned} \tag{3.5}$$

where D is any matrix fullfilling Eqs. (2.10) and $\mathbf{D}_s$ is the sth row of this matrix. We inserted Eq. (3.1) in the last line and we defined the multiple coupling coefficient (MCC) of U_n by

$$\left\langle \left[\left[\left[\begin{matrix} w_1 w_2\\ \mathbf{D}_1\mathbf{D}_2\end{matrix}\right]\begin{matrix}[g^2]w_3\\ \mathbf{D}_3\end{matrix}\right]\cdots\right]\begin{matrix}[g^{n-1}]w_n\\ \mathbf{D}_n\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle \equiv \sum_{\backslash\gamma^2/,\backslash\gamma^3/,\dots,\backslash\gamma^{n-1}/} \left\langle\begin{matrix} w_1 w_2\\ \mathbf{D}_1\mathbf{D}_2\end{matrix}\middle|\begin{matrix}[g^2]\\ \backslash\gamma^2/\end{matrix}\right\rangle\left\langle\begin{matrix}[g^2]w_3\\ \backslash\gamma^2/\mathbf{D}_3\end{matrix}\middle|\begin{matrix}[g^3]\\ \backslash\gamma^3/\end{matrix}\right\rangle\cdots\left\langle\begin{matrix}[g^{n-1}]\ w_n\\ \backslash\gamma^{n-1}/\mathbf{D}_n\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle. \tag{3.6}$$

We thus have obtained a first closed expression for double Gel'fand states. Comparing Eq. (3.5) with Eq. (2.9), we find that the coefficient $\mathbf{C}$ is exactly the MCC of Eq. (3.5).

From Eq. (3.6) and the expression given by Chacón *et al.*,[2] these coefficients are given in a closed form.

A similar expression could have been obtained by interchanging the role of rows and columns. This gives an identity between distinct MCC's that is a generalized "Regge symmetry" as shown at the end of the next section.

IV. DOUBLE GEL'FAND STATES IN TERMS OF RECOUPLING COEFFICIENTS

We now proceed to give an expression similar to (3.5), but in terms of recoupling coefficients rather than MCC. To do this, we shall show that the particular MCC (3.6) is proportional to a recoupling coefficient of the n^2 representations $D_{ij}=[D_{ij}0\cdots0]$, $i,j=1,\dots,n$. The result one obtains will have the advantage of being completely symmetric with respect to the upper and lower patterns.

We shall define a recoupling coefficient assuming that *all* couplings involved are multiplicity free.

We consider n^2 IR $[\Delta_{ij}]$ of U_n with row labels $\backslash q_{ij}/$, and we couple them in two different ways as follows:

$$\begin{aligned}&\sum_{\backslash q_1/\cdots\backslash q_n/}\prod_{i=1}^{n}\left\langle\left[\left[\left[\begin{matrix}[\Delta_{i1}][\Delta_{i2}]\\ \backslash q_{i1}/\backslash q_{i2}/\end{matrix}\right]\begin{matrix}[\sigma_i^2][\Delta_{i3}]\\ \backslash q_{i3}/\end{matrix}\right]\cdots\right]\begin{matrix}[\sigma_i^{n-1}][\Delta_{in}]\\ \backslash q_{in}/\end{matrix}\middle|\begin{matrix}[w_i]\\ \backslash q_i/\end{matrix}\right\rangle\left\langle\left[\left[\left[\begin{matrix}[w_1][w_2]\\ \backslash q_1/\backslash q_2/\end{matrix}\right]\begin{matrix}[\theta^2][w_3]\\ \backslash q_3/\end{matrix}\right]\cdots\right]\begin{matrix}[\theta^{n-1}][w_n]\\ \backslash q_n/\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle\\ &=\sum_{\substack{[\bar w_1]\ \cdots\ [\bar w_n]\\ [\bar\theta^2]\ \cdots\ [\bar\theta^{n-1}]\\ [\bar\sigma_1^2]\ \cdots\ [\bar\sigma_1^{n-1}]\\ \vdots\qquad\vdots\\ [\bar\sigma_n^2]\ \cdots\ [\bar\sigma_n^{n-1}]}}\begin{bmatrix}\Delta_{ij} & \sigma & w\\ \bar\sigma & & \theta\\ \bar w & \bar\theta & f\end{bmatrix}\sum_{\backslash\bar q_1/\cdots\backslash\bar q_n/}\prod_{j=1}^{n}\left\langle\left[\left[\left[\begin{matrix}[\Delta_{1j}][\Delta_{2j}]\\ \backslash q_{1j}/\backslash q_{2j}/\end{matrix}\right]\begin{matrix}[\bar\sigma_j^2][\Delta_{3j}]\\ \backslash q_{3j}/\end{matrix}\right]\cdots\right]\begin{matrix}[\bar\sigma_j^{n-1}][\Delta_{nj}]\\ \backslash q_{nj}/\end{matrix}\middle|\begin{matrix}[\bar w_j]\\ \backslash\bar q_j/\end{matrix}\right\rangle\\ &\quad\times\left\langle\left[\left[\left[\begin{matrix}[\bar w_1][\bar w_2]\\ \backslash\bar q_1/\backslash\bar q_2/\end{matrix}\right]\begin{matrix}[\bar\theta^2][\bar w_3]\\ \backslash\bar q_3/\end{matrix}\right]\cdots\right]\begin{matrix}[\bar\theta^{n-1}][\bar w_n]\\ \backslash\bar q_n/\end{matrix}\middle|\begin{matrix}[f]\\ \backslash\, h\,/\end{matrix}\right\rangle.\end{aligned} \tag{4.1}$$

Here we define the following compact notation for recoupling coefficients:

$$\begin{bmatrix} \Delta_{ij} & \sigma & w \\ \bar{\sigma} & & \theta \\ \bar{w} & \bar{\theta} & f \end{bmatrix} \equiv \begin{bmatrix} [\Delta_{11}] & [\Delta_{12}] & [\sigma_1^2] & [\Delta_{13}] & [\sigma_1^3] & \cdots & [\sigma_1^{n-1}] & [\Delta_{1n}] & [w_1] \\ [\Delta_{21}] & [\Delta_{22}] & [\sigma_2^2] & [\Delta_{23}] & [\sigma_2^3] & \cdots & [\sigma_2^{n-1}] & [\Delta_{2n}] & [w_2] \\ [\bar{\sigma}_1^2] & [\bar{\sigma}_2^2] & & [\bar{\sigma}_3^2] & & & & [\bar{\sigma}_n^2] & [\theta^2] \\ [\Delta_{31}] & [\Delta_{32}] & [\sigma_3^2] & [\Delta_{33}] & [\sigma_3^3] & \cdots & [\sigma_3^{n-1}] & [\Delta_{3n}] & [w_3] \\ & \cdot & & \cdot & & & & \cdot & \\ \cdot & \cdot & & \cdot & & & & \cdot & \\ \cdot & \cdot & \cdot & & & & & \cdot & \\ [\bar{\sigma}_1^{n-1}] & [\bar{\sigma}_2^{n-1}] & & [\bar{\sigma}_3^{n-1}] & & & & [\bar{\sigma}_n^{n-1}] & [\theta^{n-1}] \\ [\Delta_{n1}] & [\Delta_{n2}] & [\sigma_n^2] & [\Delta_{n3}] & [\sigma_n^3] & \cdots & [\sigma_n^{n-1}] & [\Delta_{nn}] & [w] \\ [\bar{w}_1] & [\bar{w}_2] & [\bar{\theta}^2] & [\bar{w}_3] & [\bar{\theta}] & \cdots & [\bar{\theta}^{n-1}] & [\bar{w}_n] & [f] \end{bmatrix}$$

$$= \langle \{\cdots\{(\cdots([\Delta_{11}][\Delta_{12}])[\sigma_1^2]\Delta_{13})[\sigma_1^3]\cdots[\sigma_1^{n-1}][\Delta_{1n}])[w_1](\cdots(\cdots)[w_2]\}[\theta^2]\cdots\}[\theta^{n-1}](\cdots(\cdots)[w_n]\}[f]| \tag{4.2}$$
$$\times\{\cdots\{(\cdots([\Delta_{11}][\Delta_{21}])[\bar{\sigma}_1^2]\Delta_{31})[\bar{\sigma}_1^3]\cdots[\bar{\sigma}_1^{n-1}][\Delta_{n1}])[\bar{w}_1](\cdots(\cdots)[\bar{w}_2]\}[\bar{\theta}^2]\cdots\}[\bar{\theta}^{n-1}](\cdots(\cdots)[\bar{w}_n]\}[f]\rangle.$$

The symbols $[\Delta_{ij}], [\sigma_j^i], [\bar{\sigma}_j^i], [w_i], [\bar{w}_i], [\theta^i]$, and $[\bar{\theta}^i]$ all indicate IR's of U_n; their exact roles are clear from their appearance in the MCC's.

We now proceed to identify the last MCC on the left-hand side of Eq. (4.1) with the one in (3.6). This defines all w_i to be trivial IR's $w_i = [w_i 0\cdots 0]$; the $[\Delta_{ij}]$ must, in turn, be trivial IR's of the form $D_{ij} = [D_{ij}0\cdots 0]$. The IR $[\sigma_i^j]$ then becomes spurious and may be omitted where it is convenient; the IR $[\theta^i]$ has to be choosen as $[g^i]$. The barred quantities play a similar role.

We are still free to choose the $\backslash q_{ij}/$ within certain restrictions derived from the previous choices; we shall set

$$\backslash q_{ij}/ = \begin{array}{ccc} D_{ij}0 & \cdots & 0 \\ \ddots & & \vdots \\ D_{ij}0 & \cdots & 0 \\ 0 & \cdots & 0 \\ \ddots & & \vdots \\ 0 & & \end{array} \left.\begin{array}{c} \\ \\ \\ \end{array}\right\} j-1 \quad \text{rows} \tag{4.3}$$

We now consider the first n MCC's on the right-hand side of Eq. (4.1). Employing Eq. (4.3) and notation (2.6) and (2.7), we find that the jth MCC is

$$\left\langle \left[\left[\left[\begin{matrix} D_{1j} D_{2j} \\ j \quad j \end{matrix}\right][\bar{\sigma}_j^1] \begin{matrix} D_{3j} \\ j \end{matrix}\right]\cdots\right][\bar{\sigma}_j^{n-2}]\begin{matrix} D_{nj} \\ j \end{matrix} \left| \begin{matrix} \bar{w}_j \\ \backslash \bar{q}_j / \end{matrix} \right.\right\rangle$$

$$= \delta_{\binom{\bar{w}_j}{\backslash \bar{q}_j/}, \binom{\Sigma_i D_{ij}, 0\cdots 0}{j}} \prod_{\tau=1}^{n-2} \delta_{[\sigma_j^\tau], [\Sigma_{i=1}^\tau D_{ij}, 0\cdots 0]}. \tag{4.4}$$

Thus, essentially the first n MCC's on the right-hand side are 1, the labels $\bar{w}_j$, $\bar{q}_j$, and $[\sigma_j^i]$ take the values defined in the Kronecker δ's, and the corresponding summations disappear.

Focusing now on the last MCC on the right-hand side, we find that it has the form

$$\left\langle \left[\left[\left[\begin{matrix} \bar{w}_1 \bar{w}_2 \\ 1 \quad 2 \end{matrix}\right][\bar{\theta}^2]\begin{matrix} \bar{w}_3 \\ 3 \end{matrix}\right]\cdots\right][\bar{\theta}^{n-1}]\begin{matrix} \bar{w}_n \\ n \end{matrix} \left| \begin{matrix} [f] \\ \backslash h / \end{matrix}\right.\right\rangle$$
$$= \left(\frac{\Pi_{k=1}^n \bar{w}_k! \Pi_{i<j}^n (f_i - f_j + j - i)}{\Pi_{s=1}^n (f_s + n - s)!} \right)^{1/2} \prod_{i=2}^{n-1} \delta_{[\bar{\theta}^i],[h^i]}. \tag{4.5}$$

Since in each coupling step, weight is added in one row only, beginning at the bottom, we find that for a given choice of $\backslash h /$, the $[\bar{\theta}^j]$ are fixed as indicated by the δ's, provided that the weights of $\backslash h /$ are $\bar{w}_j$; this eliminates the last sum on the right-hand side of Eq. (4.1). Furthermore, the coefficient is simple enough to be calculated using (3.6) as well as Eq. (6.2) given by Chacón *et al.*[2]; the result free of summations is given in Eq. (4.5).

We have chosen the w_i to be one-row partitions. Then the $\backslash q_i /$ are uniquely defined by the weights predetermined by the $\backslash q_{ij}/$; otherwise the coefficient becomes zero. The sum over $\backslash q_i /$ is thus eliminated, and we are left with coefficients of the type

$$\left\langle \left[\left[\left[\begin{matrix} D_{i1} D_{i2} \\ 1 \quad 2 \end{matrix}\right][\sigma_i^1]\begin{matrix} D_{i3} \\ 3 \end{matrix}\right]\cdots\right][\sigma_i^{n-2}]\begin{matrix} D_{in} \\ n \end{matrix} \left| \begin{matrix} w_i \\ q_i \end{matrix}\right.\right\rangle$$

with numerical value given by

$$\left(\prod_{i=1}^n D_{si}!/w_s!\right)^{1/2}. \tag{4.6}$$

Inserting these results in Eq. (4.1), we obtain

$$\left\langle \left[\left[\left[\begin{matrix} w_1 w_2 \\ \mathbf{D}_1 \mathbf{D}_2 \end{matrix}\right][g^2]\begin{matrix} w_3 \\ \mathbf{D}_3 \end{matrix}\right]\cdots\right][g^{n-1}]\begin{matrix} w_n \\ \mathbf{D}_n \end{matrix} \left| \begin{matrix} [f] \\ \backslash h / \end{matrix}\right.\right\rangle$$
$$= \left(\frac{\Pi_{i=1}^n w_i! \bar{w}_i! \Pi_{i<j}(f_i - f_j + j - i)}{\Pi_{s,i}^n D_{si}! \Pi_{j=1}^n (f_j + n - j)!} \right)^{1/2} \begin{bmatrix} D_{si} & & w \\ & & g \\ \bar{w} & h & f \end{bmatrix}, \tag{4.7}$$

where the trivial σ's are suppressed.

Substituting this expression into Eq. (3.5), we obtain a new closed expression for double Gel'fand states in terms of recoupling coefficients of U_n:

$$\left\langle \eta_i^s; \begin{matrix} s = 1,\dots,n \\ i = 1,\dots,n \end{matrix} \middle| \begin{matrix} / g \backslash \\ [f] \\ \backslash h / \end{matrix} \right\rangle = \left(\frac{\Pi_{k=1}^n w_k! \bar{w}_k! \Pi_{t<s}^n (f_t - f_s + s - t)}{\Pi_{j=1}^n (f_j + n - j)!} \right)^{1/2} \sum_{\mathbf{D}} \prod_{s,i=1}^n \frac{\eta_i^{s\,D_{si}}}{D_{si}!} \begin{bmatrix} D_{si} & & w \\ & & g \\ \bar{w} & h & f \end{bmatrix}. \tag{4.8}$$

Since the recoupling coefficient is invariant under reflection of the diagonal from upper left to the lower right, the result (4.8) is pleasingly symmetric with respect to upper and lower labels. Also we can take advantage of the symmetry of the recoupling coefficient in Eq. (4.7) to elucidate the following Regge symmetry for the MCC of Eq. (3.6)[13,14]:

$$\left\langle \left[\left[\begin{bmatrix} w_1 w_2 \\ \mathbf{D}_1 \mathbf{D}_2 \end{bmatrix} \begin{matrix} [g^2] w_3 \\ \mathbf{D}_3 \end{matrix} \right] \cdots \right] \begin{matrix} [g^{n-1}] w_n \\ \mathbf{D}_n \end{matrix} \middle| \begin{matrix} [f] \\ \backslash h / \end{matrix} \right\rangle = \left\langle \left[\left[\begin{bmatrix} \bar{w}_1 \bar{w}_2 \\ \mathbf{D}_1^t \mathbf{D}_2^t \end{bmatrix} \begin{matrix} [h^2] \bar{w}_3 \\ \mathbf{D}_3^t \end{matrix} \right] \cdots \right] \begin{matrix} [h^{n-1}] \bar{w}_n \\ \mathbf{D}_n^t \end{matrix} \middle| \begin{matrix} [f] \\ \backslash g / \end{matrix} \right\rangle. \tag{4.9}$$

It may also be worthwhile to note that the derivation of Eq. (4.7) actually allows for the more general case, where in the recoupling coefficient the couplings of the Δ_{ij} are stretched only in one direction, e.g., we may assume $[w_i] = [w_{i_1}, w_{i_2} \cdots w_{i_n}]$ not to be a one-row partition. In this case the generalization of Eq. (4.7) reads

$$\begin{bmatrix} \Delta_{ij} & \sigma(q) & w \\ & & \theta \\ \bar{w} & h & f \end{bmatrix} = \left[\frac{\Pi_{i,j=1}^n \Delta_{ij}! \Pi_{t=1}^n \Pi_{k<l}^n (w_{t_k} - w_{k_l} + l - k) \Pi_{s=1}^n (f_s + n - s)!}{\Pi_{i,j=1}^n (w_{i_j} + n - j)! \Pi_{k=1}^n \bar{w}_k! \Pi_{s<t}^n (f_s - f_t + t - s)} \right]^{1/2}$$
$$\times \left\langle \left[\cdots \left[\begin{matrix} [w_1][w_2] \\ \backslash q_1 / \backslash q_2 / \end{matrix} \right] \begin{matrix} [\theta^2][w_3] \\ \backslash q_3 / \end{matrix} \right] \cdots \right] \begin{matrix} [\theta^{n-1}][w_n] \\ \backslash q_n / \end{matrix} \middle| \begin{matrix} [f] \\ \backslash h / \end{matrix} \right\rangle, \tag{4.10}$$

where $\sigma(q)$ is a $n \times (n-2)$ matrix with elements $\sigma_{ij} = [(q_i)_1^j \cdots (q_i)_j^j 0 \cdots 0]$ and $(q_i)_1^j \cdots (q_i)_j^j$ means the jth row of the Gel'fand pattern $\backslash q_i /$. This expression may be useful in certain computations in nuclear physics as it provides a simple closed form for certain recoupling coefficients of SU (3) occurring in this context.[15]

V. RELATION BETWEEN RECOUPLING COEFFICIENTS FOR KRONECKER PRODUCTS IN U_n AND EXTERNAL PRODUCTS IN S_n

We shall now reinterpret the multiple recoupling coefficient of U_n obtained in the previous section as a recoupling coefficient for external products in S_n.

Any multiplicities that may occur in such products are completely equivalent (see, e.g., Hamermesh[16]). Since the actual problem at hand is multiplicity-free, we omit all multiplicity labels, but we note that the entire argument is valid if nontrivial multiplicities occur. In the previous section the simple relation between MCC's and recoupling coefficients depends on the particular form of the IR involved. The relation we derive next between recoupling coefficients of S_n and U_n will be general, despite the fact that we shall apply it to the particular case of the previous section.

A special Gel'fand state is defined to be a double Gel'fand state, *one* of whose weights is $(1,1,\dots,1)$. Given this weight, two consecutive rows in the Gel'fand patterns differ in just one label; accordingly, the Gel'fand pattern may be characterized by a Yamanouchi symbol or, equivalently, by a Young tableau. We shall abbreviate such a Yamanouchi symbol by a Greek label μ; thus

$$\left\langle \eta_i^s; \begin{matrix} s = 1,\dots,n \\ i = 1,\dots,n \end{matrix} \middle| f; \begin{matrix} \mu \\ \backslash g / \end{matrix} \right\rangle$$

will denote a special Gel'fand state where the particular weight corresponding to μ is realized for the upper pattern. We can now choose the subgroup S_n of $\mathscr{U}_n$ that permutes the weights. The special Gel'fand states will span an invariant subspace under this subgroup; indeed, it can be shown that they form a Yamanouchi basis for the IR f of S_n.[4]

(Actually, the concept of special states is not restricted to the relation between a Gel'fand and a Yamanouchi basis. For example, a Weyl basis of U_n will go into a basis for the rational representation of S_n in an analogous fashion,[17] and we can generally speak of special states to establish relations between bases of U_n and S_n.)

Consider now the subsets $\underline{N}_{ij}$ of the ordered set $\underline{N}$ and the two chains of groups

$$S_N \supset S_{N-\underline{N}_1} \times S_{\underline{N}_1} \supset \cdots \supset \prod_{i=1}^n S_{\underline{N}_i},$$
$$S_{\underline{N}_i} \supset S_{\underline{N}_i - \underline{N}_{i1}} \times S_{\underline{N}_{i1}} \supset \cdots \supset \prod_{j=1}^n S_{\underline{N}_{ij}}, \tag{5.1}$$
$$S_N \supset S_{N-\bar{\underline{N}}_1} \times S_{\bar{\underline{N}}_1} \supset \cdots \supset \prod_{j=1}^n S_{\bar{\underline{N}}_j},$$
$$S_{\bar{\underline{N}}_j} \supset S_{\bar{\underline{N}}_j - \underline{N}_{1j}} \times S_{\underline{N}_{1j}} \supset \cdots \supset \prod_{i=1}^n S_{\underline{N}_{ij}}, \tag{5.2}$$

where $\underline{N}_i = \cup_{j=1}^n \underline{N}_{ij}$, $\bar{\underline{N}}_j = \cup_{i=1}^n \underline{N}_{ij}$ and where, e.g., $S_{\underline{N}_{ij}}$ is the group of permutations of the elements in the set $\underline{N}_{ij}$.

Note that the last groups in both chains, $\Pi_{i=1}^n \Pi_{j=1}^n S_{\underline{N}_{ij}}$ and $\Pi_{j=1}^n \Pi_{i=1}^n S_{\underline{N}_{ij}}$, are conjugate and connected by the permutation

$$\begin{pmatrix} \underline{N}_{11} & \underline{N}_{12} & \cdots & \underline{N}_{1n} & \underline{N}_{21} & \cdots & \underline{N}_{nn} \\ \underline{N}_{11} & \underline{N}_{21} & \cdots & \underline{N}_{n1} & \underline{N}_{12} & \cdots & \underline{N}_{nn} \end{pmatrix} = Z,$$

which is to be interpreted as replacing each set by the corresponding string of numbers.[9]

We now define a recoupling coefficient for the outer product of S_n as the matrix element of Z between a bra that is subduced according to the chain (5.1) and a ket that is subduced according to the chain (5.2):

$$\langle [\cdots [(\cdots(\Delta_{11}\Delta_{12})\gamma_1^1 \Delta_{13})\gamma_1^2 \cdots \Delta_{1n})w_1(\cdots(\Delta_{21}\Delta_{22})\gamma_2^1 \cdots \Delta_{2n})w_2]$$
$$\times \theta_2 \cdots \theta_{n-1}(\cdots)w_n]\alpha | Z | [\cdots[((\cdots(\Delta_{11}\Delta_{21})\bar{\gamma}_1^1 \Delta_{31})\bar{\gamma}_1^2 \cdots \Delta_{n1})$$
$$\times \bar{w}_1(\cdots(\Delta_{12}\Delta_{22})\bar{\gamma}_2^1 \cdots \Delta_{n2})\bar{w}_2]\bar{\theta}_2 \cdots \bar{\theta}_{n-1}(\cdots)\bar{w}_n]\alpha \rangle,$$

where the Δ_{ij} are the IR's of $S_{\underline{N}_{ij}}$. The symbols γ_i^j, (5.3)

$\bar{\gamma}_j^i$, w_i, $\bar{w}_i$, θ_i, and $\bar{\theta}_i$ are IR's of the subgroups $S_{N_{1j}+\cdots+N_{ij+1}}$, $S_{N_{ij}+\cdots+N_{i+1j}}$, S_{N_i}, $S_{\bar{N}_i}$, $S_{N_1+\cdots+N_i}$, and $S_{\bar{N}_1+\cdots+\bar{N}_i}$, respectively. The row labels of Δ_{ij} do not appear and the matrix elements are diagonal in Δ_{ij}, since the sets N_{ij} are permuted without suffering internal reordering.

We may now calcuate this coefficient by taking the matrix element of a weight permutation between special states that transform like the bra and ket, respectively.

We proceed, e.g., to construct the state for the ket, coupling successively with respect to U_N. Using arguments similar to those that lead to Eq. (3.5), we find:

$$\left\langle \eta_i^s;\ \begin{matrix} s\in N \\ t=1,\ldots,n \end{matrix} \middle| \alpha\setminus q/;\left\{\cdots\left\{\left[\cdots\begin{bmatrix}\Delta_{11} & \Delta_{21}\\ \tau_{11} & \tau_{21}\end{bmatrix}^{\bar{\gamma}_1^1}\cdots\right]^{\bar{\gamma}_1^{n-2}} \begin{matrix}\Delta_{n1}\\ \tau_{n1}\end{matrix}\right]^{\bar{w}_1}\left[\cdots\left[\cdots\right]^{\bar{w}_2}\right\}^{\bar{\theta}_2}\cdots\right\}^{\bar{\theta}_{n-1}}\left[\cdots\left[\cdots\right]^{\bar{w}_n}\right\}^{\alpha}\right\rangle$$

$$= \sum_{\substack{q_{11},q_{12},\ldots,q_{nn}\\ \bar{q}_1,\ldots,\bar{q}_n}} \prod_{i=1}^{n}\left\langle\left[\cdots\begin{bmatrix}\Delta_{1i} & \Delta_{2i}\\ q_{1i} & q_{2i}\end{bmatrix}^{\bar{\gamma}_1^i} \begin{matrix}\Delta_{3i}\\ q_{3i}\end{matrix}\right]^{\bar{\gamma}_2^i}\cdots\right]^{\bar{\gamma}_n^{i-2}} \begin{matrix}\Delta_{ni}\\ q_{ni}\end{matrix}\left|\begin{matrix}\bar{w}_i\\ \bar{q}_i\end{matrix}\right\rangle\left\langle\left[\cdots\begin{bmatrix}\bar{w}_1 & \bar{w}_2\\ \bar{q}_1 & \bar{q}_2\end{bmatrix}^{\bar{\theta}_2} \begin{matrix}\bar{w}_3\\ \bar{q}_3\end{matrix}\right]^{\bar{\theta}_3}\cdots\right]^{\bar{\theta}_{n-1}} \begin{matrix}\bar{w}_n\\ \bar{q}_n\end{matrix}\left|\begin{matrix}\alpha\\ \setminus q/\end{matrix}\right\rangle$$

$$\times \prod_{j=1}^{n}\left\langle \eta_j^s;\ \begin{matrix} s\in N_{ji} \\ t=1,\ldots,n \end{matrix}\middle|\Delta_{ji};\begin{matrix}\tau_{ji}\\ q_{ji}\end{matrix}\right\rangle. \tag{5.4}$$

Note that with respect to the upper labels we have a special state that is part of a basis of an IR for the permutation group of the weights and of the form required in Eq. (5.3).

In the matrix element between such states, the permutation acts trivially on the product of uncoupled kets. Clearly the scalar product is diagonal in the IR labels Δ_{ij} and in the row labels q_{ij} of $S_{N_{ij}}$, and is independent of the latter labels. Since all states are normalized, we obtain

$$\left\langle \alpha\setminus q/;\left\{\cdots\left\{\left[\begin{bmatrix}\Delta_{11} & \Delta_{12}\\ \tau_{11} & \tau_{12}\end{bmatrix}^{\gamma_1^1}\cdots\right]^{\gamma_1^{n-2}} \begin{matrix}\Delta_{1n}\\ \tau_{1n}\end{matrix}\right\}^{w_1}\right\}^{\theta_{n-1}}\left[\cdots\left[\cdots\right]^{\bar{w}_n}\right\}^{\alpha}\middle| Z \middle| \alpha\setminus q/;\left\{\cdots\left\{\left[\begin{bmatrix}\Delta_{11} & \Delta_{21}\\ \tau_{11} & \tau_{21}\end{bmatrix}^{\bar{\gamma}_1^1}\cdots\right]^{\bar{\gamma}_1^{n-1}} \begin{matrix}\Delta_{n1}\\ \tau_{n1}\end{matrix}\right\}^{\bar{w}_1}\cdots\right\}^{\bar{\theta}_{n-1}}\left[\left[\cdots\right]^{\bar{w}_n}\right\}^{\alpha}\right\rangle$$

$$= \sum_{\substack{q_{11},q_{12},\ldots,q_{nn}\\ \bar{q}_1,\ldots,\bar{q}_n\\ q_1,\ldots,q_n}} \left\langle\left[\left[\begin{bmatrix}w_1 & w_2\\ q_1 & q_2\end{bmatrix}^{\theta_2} \begin{matrix}w_3\\ q_3\end{matrix}\right]^{\theta_3}\cdots\right]^{\theta_{n-1}} \begin{matrix}w_n\\ q_n\end{matrix}\left|\begin{matrix}\alpha\\ \setminus q/\end{matrix}\right\rangle \prod_{j=1}^{n}\left\langle\left[\left[\begin{bmatrix}\Delta_{j1} & \Delta_{j2}\\ q_{j1} & q_{j2}\end{bmatrix}^{\gamma_1^j} \begin{matrix}\Delta_{j3}\\ q_{j3}\end{matrix}\right]^{\gamma_2^j}\cdots\right]^{\gamma_{n-2}^j} \begin{matrix}\Delta_{jn}\\ q_{jn}\end{matrix}\left|\begin{matrix}w_j\\ q_j\end{matrix}\right\rangle$$

$$\times\left\langle\left[\left[\begin{bmatrix}\Delta_{1j} & \Delta_{2j}\\ q_{1j} & q_{2j}\end{bmatrix}^{\bar{\gamma}_1^j} \begin{matrix}\Delta_{3j}\\ q_{3j}\end{matrix}\right]^{\bar{\gamma}_2^j}\cdots\right]^{\bar{\gamma}_{n-2}^j} \begin{matrix}\Delta_{nj}\\ q_{nj}\end{matrix}\left|\begin{matrix}\bar{w}_j\\ \bar{q}_j\end{matrix}\right\rangle\left\langle\left[\left[\begin{bmatrix}\bar{w}_1 & \bar{w}_2\\ \bar{q}_1 & \bar{q}_2\end{bmatrix}^{\bar{\theta}_2} \begin{matrix}\bar{w}_3\\ \bar{q}_3\end{matrix}\right]^{\bar{\theta}_3}\cdots\right]^{\bar{\theta}_{n-1}} \begin{matrix}\bar{w}_n\\ \bar{q}_n\end{matrix}\left|\begin{matrix}\alpha\\ \setminus q/\end{matrix}\right\rangle \tag{5.5}$$

In the right-hand side we have a sum over Clebsch–Gordan coefficients of U_N; this sum defines a recoupling coefficient of this group as may be confirmed by comparing with Eq. (4.1), after using unitarity relations for the MCC's to gather them on one side of the equality.

Therefore, we finally have the relation

$$\begin{bmatrix}
\Delta_{11} & \Delta_{12} & \gamma_1^1 & \Delta_{13} & \gamma_1^2 & \cdots & \gamma_1^{n-2} & \Delta_{1n} & w_1\\
\Delta_{21} & \Delta_{22} & \gamma_2^1 & \Delta_{23} & \gamma_2^2 & \cdots & \gamma_2^{n-2} & \Delta_{2n} & w_2\\
\bar{\gamma}_1^1 & \bar{\gamma}_2^1 & & \bar{\gamma}_3^1 & & & & \bar{\gamma}_n^1 & \theta_2\\
\Delta_{31} & \Delta_{32} & \gamma_3^1 & \Delta_{33} & \gamma_3^2 & \cdots & \gamma_3^{n-2} & \Delta_{3n} & w_3\\
\cdot & \cdot & & \cdot & & & & \cdot & \cdot\\
\cdot & \cdot & & \cdot & & & & \cdot & \cdot\\
\cdot & \cdot & & \cdot & & & & \cdot & \cdot\\
\bar{\gamma}_1^{n-2} & \bar{\gamma}_2^{n-2} & & \bar{\gamma}_3^{n-2} & & & & \bar{\gamma}_n^{n-2} & \theta_{n-1}\\
\Delta_{n1} & \Delta_{n2} & \gamma_n^1 & \Delta_{n3} & \gamma_n^2 & \cdots & \gamma_n^{n-2} & \Delta_{nn} & w_n\\
\bar{w}_1 & \bar{w}_2 & \bar{\theta}_2 & \bar{w}_3 & & \cdots & \bar{\theta}_{n-1} & \bar{w}_n & \alpha
\end{bmatrix}
\begin{aligned}
&= \langle[\cdots[(\cdots(\Delta_{11}\Delta_{12})\gamma_1^1\Delta_{13})\gamma_1^2\cdots\Delta_{1n})w_1(\cdots)w_2]\theta_2\cdots]\theta_{n-1}(\cdots)w_n]\alpha\\
&\times|Z|[\cdots[(\cdots(\Delta_{11}\Delta_{21})\bar{\gamma}_1^1\Delta_{31})]\bar{\gamma}_1^2\cdots\Delta_{n1})\bar{w}_1(\cdots)\bar{w}_2]\bar{\theta}_2\cdots]\bar{\theta}_{n-1}(\cdots)\bar{w}_n]\alpha\rangle
\end{aligned} \tag{5.6}$$

Thus step C of Fig. 1 is completed. Step D is proved directly,[5] essentially by using matrix basis elements of S_N applied to the indices of a simple product of states of creation operators or (equivalently) of Bargmann space variables. A mistake in the normalization given in Ref. 5 is corrected in the Appendix.

VI. CONCLUSION

Closed forms for double Gel'fand states have been derived by straightforward methods of vector coupling in U_n and related to different results previously obtained. It is important to note that the coefficients involved are available explicitly in terms of factorials.

The main feature of the train of thought followed is that it yields, in a simple and straightforward way, deep insight into the structure of Gel'fand states. The use of boson polynomials is convenient but by no means essential to the arguments given.

The practical importance of these results consists of relating certain coefficients of S_N that appear frequently in problems involving the evaluation of matrix elements of antisymmetric states[18] to multiple Clebsch–Gordan coefficients of U_N, which may be evaluated following Chacón *et al.*[2]

Finally, this paper establishes implicitly the relation between the unitary and the permutation group approaches to the evaluation of matrix elements between antisymmetrized states.[18,19]

APPENDIX

From Ref. 5, Eq. 10.5 we take the following expression for the normalization constant (we drop the square-root of the denominator given there erroneously):

$$N=\left[\sum_k \frac{\langle \alpha\bar{\theta}E(\bar{H})|Z_k|\alpha\theta E(H)\rangle^2}{\Pi_{i,j}^n[\Delta_{ij}(Z_k)]!}\right]^{-1/2}. \tag{A1}$$

The symbols are as in Sec. V except that the identity IR of $S_{w_1}\times S_{w_2}\times\cdots\times S_{w_n}=H$ is abbreviated by $E(H)$ and similarly $E(\bar{H})$.

The expression (A1) may be summed as a particular case of an orthonormality relation for double coset coefficients obtained by Klein *et al.*[18] Considering such expressions, we have

$$\sum_k (1/d_k)\langle \alpha\bar{\theta}E(\bar{H})|Z_k|\alpha\theta E(H)\rangle\langle \alpha'\bar{\theta}'E(\bar{H}')|Z_k|\alpha'\theta'E(H')\rangle$$
$$=\frac{n!}{|\bar{H}||H||\alpha|}\delta_{\alpha,\alpha'}\delta_{E(\bar{H}),E(\bar{H}')}\delta_{E(H),E(H')}, \tag{A2}$$

where d_k denotes the number of times a double coset $\bar{H}Z_kH$ is covered by $\bar{h}Z_kh$ as h and $\bar{h}$ range over H and $\bar{H}$ respectively, it is given by $\Pi_{i,j}^n[D_{ij}(Z_k)]!$. $|\alpha|$ means the order of the IR α, and $|H|$ and $|\bar{H}|$ indicate the order of H and $\bar{H}$.

From (A1) and (A2) it follows that

$$\sum_k \frac{\langle \alpha\theta E(H)|Z_k|\alpha\theta E(H)\rangle^2}{\Pi_{i,j}^n[D_{ij}(Z_k)]!}=\frac{n!}{|\bar{H}|\ |\alpha|\ |H|}. \tag{A3}$$

Substituting the corresponding values for $|\alpha|$,[20] $|H|$, and $|\bar{H}|$, we have for the normalization constant

$$N=\left[\frac{\Pi_{i=1}^n\bar{w}_i!w_i!\Pi_{i<j}^n(f_i-f_j+j-i)}{\Pi_{i=1}^u(f_i+n-i)!}\right]^{1/2}. \tag{A4}$$

Using this constant, the results in Ref. 5 and Sec. V coincide.

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Geometric quantization and UIR's of semisimple Lie groups. II. Discrete series

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The Auslander–Kostant induction scheme is extended to yield the discrete series UIR's of G (G semisimple) in the L^2-cohomology group $\mathscr{H}^i_0(\mathscr{L}_\lambda)$, where $i = \frac{1}{2}(\dim k - \operatorname{rank} g)$ or $i = \frac{1}{2}\dim p$. We show that this involves a choice of complex structure in each Weyl chamber which is intimately connected with the choice of a positive polarization at that point. We illustrate our results with the example of Spin (4,2).

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I. INTRODUCTION

The intimate connection between the Auslander–Kostant theory of UIR's of simply connected solvable Lie groups[1] and the geometric quantization scheme[2] is very well known. Here, we continue to analyze the UIR's of semisimple Lie groups with special emphasis on the discrete series representation. We know from Schmid's work[3] that for all semisimple G with compact Cartan subgroup H, the discrete series UIR's are realized in $\mathscr{H}^i_0(\mathscr{L}_\lambda)$, the Hilbert space of i-forms which are solutions of the Laplace–Beltrami equation

$$\Box\omega = 0. \tag{I.1}$$

We note that in Schmid's theory the degree i of the form is dependent on the Weyl chamber in which the character e^λ defining the representation lies. In a previous paper,[4] we have shown that for Spin (2,1) and Spin (2,2), it is possible to choose complex structures in each Weyl chamber in such a manner that $i = 0$, leading to UIR's in Hilbert spaces of functions rather than forms. We also showed that this choice of complex structure is very naturally tied up with the choice of a positive polarization in the Auslander–Kostant theory. Finally, it was clear from our analysis that if $i = 0$, then Auslander–Kostant theory was sufficient to reproduce all the well-known results.

Our aim in this paper is to generalize the above analysis to arbitrary semisimple Lie groups, and to extend the Auslander–Kostant induction scheme in order that it may yield the discrete series UIR's. Our results can be summarized by the following

Theorem: Let G be semisimple. Let H be a compact Cartan subgroup of G. Then, to each nonsingular $\lambda\in h^*_c$ (the complex dual of h_c) leading to a character e^λ on H, there corresponds a unique element $s\in h$ which is regular and quantizable in the sense of Kostant. Further, there exists a positive polarization $\mathscr{S}_x$ at x. Choosing complex structures on G/H in accordance with the choice of $\mathscr{S}_x$, all discrete series UIR's of G appear in spaces $\mathscr{H}^i_0(\mathscr{L}_\lambda)$, where

$$i = \tfrac{1}{2}(\dim k - \dim h) \quad \text{or} \quad i = \tfrac{1}{2}\dim p, \tag{I.2}$$

$g = k + p$ being the Cartan decomposition.

We give the proof of this theorem in Sec. II. We illustrate the theorem with the example of a physically important group, Spin (4,2), in Sec. III.

Throughout this paper, we assume that G has discrete series representations.

II. GENERAL THEORY AND PROOF OF THE THEOREM

Let G be a semisimple Lie group with g as its Lie algebra. Let H be a compact Cartan subgroup and let h be its Lie algebra. We define a mapping

$$j = h \to h^*_c \quad \text{(the complex dual of } h_c)$$

by $x \mapsto \lambda$, $h_\lambda = 2\pi i x$, where

$$\lambda(h) = B(h_\lambda, h) \quad \forall h\in h_c. \tag{II.1}$$

Let $\mathscr{L} = \{\lambda\in h^*_c : e^\lambda \text{ is a character on } H\}$.

Proposition 1: $x\in h$ is quantizable iff $j(x)\in\mathscr{L}$. Define the scalar product

$$(\lambda,\alpha) = B(h_\lambda, h_\alpha), \quad \lambda,\alpha\in h^*_c. \tag{II.2}$$

Let Δ be the system of roots associated with (g, h) and define

$$\tilde{\omega}(\lambda) = \prod_{\alpha\in\Delta}(\lambda,\alpha) \quad \forall\lambda\in h^*_c. \tag{II.3}$$

Let

$$\mathscr{L}' = \{\lambda\in\mathscr{L} : \tilde{\omega}(\lambda)\neq 0\}. \tag{II.4}$$

Lemma 1: The following statements are equivalent: (i) $x\in h$ is regular and quantizable and (ii) $j(x)\in\mathscr{L}'$.

Proof: This follows from

$$(\lambda,\alpha) = B(h_\lambda, h_\alpha) = \alpha(h_\lambda) = 2\pi i\alpha(x), \tag{II.5}$$

where $\lambda = j(x)$. Note, of course, that if $\alpha(x) = 0$ for some $\alpha\in\Delta$, then $g_\alpha + g_{-\alpha} \subseteq g_x$ and hence x is not regular.

Let $\mathscr{S}_x$ be a positive polarization at x.

Lemma 2: (i) $\mathscr{S}_x$ exists for all regular x and is of the form

$$\mathscr{S}_x = h + n', \quad n' = \{g_\alpha : \alpha\in\Delta'\}, \tag{II.6}$$

where Δ' is a certain subspace of Δ.

$$\text{(II)}\ \alpha\in\Delta' \Leftrightarrow (\lambda,\alpha) > 0, \quad \text{where } \lambda = j(x). \tag{II.7}$$

Proof: The existence and general form of $\mathscr{S}_x$ is well known.[5] To prove (ii), let $\{h_i\}$ be a basis of h such that

$$B(h_i, h_j) = -\delta_{ij}. \tag{II.8}$$

Since H is compact all the roots are pure imaginary on h. It follows immediately that

$$h_\alpha = -i\sum(\alpha_k)h_k,$$

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where (α_k) is defined by

$$i(\alpha_k) = \alpha(h_k), \quad (\alpha_k)\in\mathbb{R}. \tag{II.9}$$

Since H is compact, it is easy to show that

$$\lambda\in\mathscr{L}\Rightarrow\lambda = \sum_\alpha n_\alpha \alpha, \quad n_\alpha\in\mathbb{Z}, \tag{II.10}$$

implying $h_\lambda = -i\sum_k(\lambda_k)h_k$ and

$$(\lambda,\alpha) = B(H_\lambda,H_\alpha) = \sum_k(\alpha_k)(\lambda_k). \tag{II.11}$$

Finally, if $z\in\mathfrak{g}_\alpha$, then

$$[\bar{z},z] = -i\gamma\sum_k(\alpha_k)h_k, \quad \gamma\in\mathbb{R}, \gamma>0. \tag{II.12}$$

Defining $\lambda = j(x)$, one has

$$\begin{aligned} &iB(x,\{\bar{z},z\}\geqslant 0\Leftrightarrow -\sum_{k,l}\mathrm{B}((\lambda_k)h_k,(\alpha_l)h_l\geqslant 0 \\ &\Leftrightarrow -B(h_i,h_j)(\lambda,\alpha)\geqslant 0\Leftrightarrow(\lambda,\alpha)\geqslant 0. \end{aligned} \tag{II.13}$$

From the fact that the α's are pure imaginary, we conclude that $\mathfrak{n}'\cap\mathfrak{g} = 0$. Also, we know that $\overline{\mathfrak{g}_\alpha} = \mathfrak{g}_{-\alpha}$.

Hence,

$$\delta = \mathfrak{g}\cap\mathscr{S}_x = \mathfrak{h}, \quad e = \mathfrak{g}\cap(\mathscr{S}_x + \overline{\mathscr{S}}_x) = \mathfrak{g}. \tag{II.14}$$

Define

$$\Delta_{\mathfrak{k}}^{\pm}(x) = \{\alpha\in\Delta:\mathfrak{g}_{\pm\alpha}\subseteq\mathscr{S}_x\}. \tag{II.15}$$

Since $\mathscr{S}_x$ is a polarization and hence isotropic with respect to B, it follows immediately that $\Delta_{\mathfrak{k}}^{\pm}(x)$ is a positive (resp. negative) subspace of Δ and therefore can be used in place of the Δ^+ used by Schmid.

Define

$$\begin{aligned} K_{\mathfrak{k}}^{\pm}(\lambda) = \mathrm{card}\{&\alpha\in\Delta_{\mathfrak{k}}^{\pm}(x),\mathfrak{g}_\alpha\subseteq\mathfrak{k}_c, (\lambda,\alpha)<0\} \\ &+ \mathrm{card}\{\alpha\in\Delta_{\mathfrak{k}}^{\pm}, \mathfrak{g}_\alpha\subseteq\mathfrak{p}_c, (\lambda,\alpha)>0\}, \end{aligned} \tag{II.16}$$

where $\lambda = j(x)$. It follows immediately from Lemma 2 that

$$\begin{aligned} K_{\mathfrak{k}}^{+}(\lambda) &= \mathrm{card}\{\alpha\in\Delta^+(x):\mathfrak{g}_\alpha\subseteq\mathfrak{p}_c\} = \tfrac{1}{2}\dim\mathfrak{p}, \\ K_{\mathfrak{k}}^{-}(\lambda) &= \mathrm{card}\{\alpha\in\Delta^-(x):\mathfrak{g}_\alpha\subseteq\mathfrak{k}_c\} \\ &= \tfrac{1}{2}(\dim\mathfrak{k} - \dim\mathfrak{h}) = \tfrac{1}{2}(\dim\mathfrak{k} - \mathrm{rank}\,\mathfrak{g}). \end{aligned} \tag{II.17}$$

Using the results of Schmid, we now conclude that the spaces $\mathscr{H}_0^i(\mathscr{L}_\lambda)$, $i = K_{\mathfrak{k}}^{\pm}(\lambda)$ depending on the choice of positive subspace of Δ, bear UIR's of G, proving the theorem stated in Sec. I.

Corollary: Let G be compact. Then the discrete series of UIR's appear in spaces of holomorphic function (i.e., $K_{\mathrm{k}}^{+}(\lambda) = 0$).

We know that all compact Cartan subalgebras of $\mathfrak{g}$ are equivalent to one another. Also, every regular $x\in\mathfrak{k}$ belongs to a unique compact Cartan subalgebra. Now, from Schmid's work, we know that the discrete series UIR's derived by choosing different compact Cartan subgroups are equivalent. We thus have the following

Theorem 2: Let $x\in\mathfrak{k}$ be regular, semisimple, and quantizable. Let $\mathscr{S}_x$ be a positive polarization at x. Let e^λ denote the character whose differential is given by $2\pi iB(x,-)$. Let D, E be constructed as usual and let $\mathscr{A}_0^i(\mathscr{L}_\lambda)$ be the space of i – forms with compact support on the line bundel $\mathscr{L}_\lambda$ associated with the principal bundle $D\rightarrow E\rightarrow E/D$ and let $\mathscr{H}_0^i(\mathscr{L}_\lambda)$ be defined in terms of $\mathscr{A}_0^i(\mathscr{L}_\lambda)$ as in Schmid with i given by Eq. (II.17). Let $\widetilde{\mathrm{ind}}_D^E(e^\lambda)$ denote the natural representation at G or $\mathscr{H}_0^i(\mathscr{L}_\lambda)$. Then

$$\sigma = \mathrm{ind}_E^G(\widetilde{\mathrm{ind}}_D^E e^\lambda) \tag{II.18}$$

is irreducible and is dependent only on the orbit of x under $\mathrm{Ad}\mathfrak{k}$.

The formal similarity between this result and the result of Auslander–Kostant is worth noting. Of course, if $i = 0$ (e.g., for G compact) then the induction scheme reduces to the Auslander–Kostant scheme.

III. APPLICATION TO SPIN (4,2)

We define the Lie algebra SO(4,2) by

$$[J_{ij},J_{kl}] = g_{ik}J_{jl} + g_{jl}J_{ik} - g_{il}J_{jk} - g_{jk}J_{il}, J_{ij} = -J_{ji}.$$

where $i,j = 1,\ldots,6$ and

$$\mathrm{g}_{ij} = \mathrm{diag}\{+1,+1,+1,+1,-1,-1\}. \tag{III.1}$$

B is defined by

$$B(J_{ij},J_{kl}) = -(g_{ik}g_{jl} - g_{il}g_{jk}),$$

with

$$\begin{aligned} \mathfrak{k} &= \{J_{12},J_{13},J_{14},J_{23},J_{24},J_{34},J_{56}\}, \\ \mathfrak{p} &= \{J_{15},J_{25},J_{35},J_{45},J_{16},J_{26},J_{36},J_{46}\}. \end{aligned} \tag{III.2}$$

$\mathfrak{h}$ can be chosen as

$$\mathfrak{h} = \{J_{12},J_{34},J_{56}\}. \tag{III.3}$$

It follows immediately that $K_{\mathfrak{k}}^{+}(\lambda) = 4$, $K_{\mathfrak{k}}^{-}(\lambda) = 2$. $(\mathfrak{g},\mathfrak{h})$ has twelve roots:

$$\begin{aligned} &\alpha_1 = (i,-i,0) && \mathfrak{g}_{\alpha_1} = \{J_{13} + iJ_{23} - i(J_{24} + iJ_{34})\}\in\mathfrak{k}_c, \\ &\alpha_2 = (0,i,i) && \mathfrak{g}_{\alpha_2} = \{J_{35} + iJ_{45} + i(J_{36} + iJ_{46})\}\in\mathfrak{p}_c, \\ &\alpha_3 = (0,i,-i) && \mathfrak{g}_{\alpha_3} = \{J_{35} + iJ_{45} - i(J_{36} + iJ_{46})\}\in\mathfrak{p}_c, \\ &\alpha_4 = (i,i,0) && \mathfrak{g}_{\alpha_4} = \{J_{13} + iJ_{23} + i(J_{24} + iJ_{34})\}\in\mathfrak{k}_c, \\ &\alpha_5 = (i,0,i) && \mathfrak{g}_{\alpha_5} = \{J_{15} + iJ_{25} + iJ_{16} + iJ_{26})\}\in\mathfrak{p}_c, \\ &\alpha_6 = (i,0,-i) && \mathfrak{g}_{\alpha_6} = \{J_{15} + iJ_{25} - i(J_{16} + iJ_{26})\}\in\mathfrak{p}_c, \end{aligned} \tag{III.4}$$

where, e.g., $\alpha_1 = (i,-i,0)$ means that

$$\alpha_1(J_{12}) = -\alpha_1(J_{34}) = i, \alpha_1,(J_{56}) = 0,$$

and where

$$\mathfrak{g}_{-\alpha} = \overline{\mathfrak{g}_\alpha}.$$

It is easy to see that if

$$\lambda = \lambda_1\alpha_1 + \lambda_2\alpha_2 + \lambda_3\alpha_3,$$

then

$$\lambda = (i\lambda_1, i(\lambda_2 + \lambda_3 - \lambda_1), i(\lambda_2 - \lambda_3)). \tag{III.5}$$

It follows therefore that

$$\mathscr{L} = \{\lambda = n_1\alpha_1 + n_2\alpha_2 + n_3\alpha_3,\ n_1,n_2,n_3\in\mathbb{Z}\}. \tag{III.6}$$

$\tilde{\omega}(\lambda)\neq 0$ imposes six conditions on λ:

$$\begin{aligned} &\text{(i)}\ 2\mathrm{n}_1 - \mathrm{n}_2 - \mathrm{n}_3\neq 0, && \text{(ii)}\ 2\mathrm{n}_2 - \mathrm{n}_1\neq 0, \\ &\text{(iii)}\ 2\mathrm{n}_3 - \mathrm{n}_1\neq 0, && \text{(iv)}\ \mathrm{n}_2 + \mathrm{n}_3\neq 0, \\ &\text{(v)}\ \mathrm{n}_1 + \mathrm{n}_2 - \mathrm{n}_3\neq 0, && \text{(vi)}\ \mathrm{n}_1 - \mathrm{n}_2 + \mathrm{n}_3\neq 0, \end{aligned} \tag{III.7}$$

corresponding to the six conditions $(\lambda,\alpha_i)\neq 0$. These six con-

TABLE I. Subspaces of $\mathscr{L}'$ classified by sign of (λ,α_i), $i = 1,\ldots,6$ and corresponding values of $K_s(\lambda)$.

S.No.	Sign of (λ,α_i), $i = 1,\ldots,6$ 1	2	3	4	5	6	$K_s(\lambda)$
1	+	+	+	+	+	+	2
2	+	+	−	+	+	+	3
3	+	+	−	+	+	−	4
4	+	+	−	−	+	−	3
5	+	−	+	+	+	+	3
6	+	−	+	−	−	+	4
7	+	−	+	−	−	+	3
8	+	−	−	+	+	+	4
9	+	−	−	+	+	+	3
10	+	−	−	+	+	−	4
11	+	−	−	−	−	+	4
12	+	−	−	−	−	−	5
13	−	+	+	+	+	+	1
14	−	+	+	+	+	−	2
15	−	+	+	−	−	+	2
16	−	+	+	−	−	−	3
17	−	+	+	−	−	−	2
18	−	+	−	+	+	−	3
19	−	+	−	+	+	−	2
20	−	+	−	−	−	−	3
21	−	−	+	−	−	+	3
22	−	−	+	−	−	+	2
23	−	−	+	−	−	−	3
24	−	−	−	−	−	−	4

ditions are not always independent, e.g., if $2n_1 - n_2 - n_3 > 0$, $2n_2 - n_1 > 0$, then $n_1 + n_2 - n_3 > 0$. One accordingly gets 24 subspaces of $\mathscr{L}'$, where two subspaces are distinguished by the signs of the (λ,α_i). These subspaces are listed in Table I, where the entry under i is the sign of (λ,α_i). Note here, that, e.g., $(\lambda,\alpha_1) > 0 \Rightarrow 2n_1 - n_2 - n_3 < 0$. Also listed for each case is the value of $K_s(\lambda)$, defined with reference to $\Delta^+ = \{\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5,\alpha_6\}$. Note that $K_s(\lambda)$ varies from subspace to subspace. The positive polarizations attached to each x can be read off from the same table, using Lemma 2. For example, for case 1, where all $(\lambda\alpha_i) > 0$, one has

$$\mathscr{S}_x = \not{h} + \mathscr{g}_{\alpha_1} + \mathscr{g}_{\alpha_2} + \mathscr{g}_{\alpha_3} + \mathscr{g}_{\alpha_4} + \mathscr{g}_{\alpha_5} + \mathscr{g}_{\alpha_6}. \quad \text{(III.8)}$$

Forming $\Delta_k^{\pm}(x)$, one gets

$$\Delta_k^+(x) = \Delta^+, \quad \Delta_k^-(x) = \Delta - \Delta^+, \quad \text{(III.9)}$$

and hence $K_k^+(\lambda) = 4$, $K_k^-(\lambda) = 2$ as expected.

IV. CONCLUSIONS

By choosing different complex structures in different Weyl chambers of $\not{h}_c^*$, we have shown that the Schmid representations are realizable in $\mathscr{H}_0^i(\mathscr{L}_\lambda)$, where i is constant over the Weyl chambers. In particular, for G compact, we have seen that it is possible to choose $i = 0$, which reproduces the classical results. We note also that our choice of complex structure at each point x is intimately related to the choice of a positive polarization at that point. This result encourages us to believe that the Auslander–Kostant theory could be extended to semisimple Lie groups.

There are, of course, at least two problems to be solved before such an extension can be performed.

(1) The parameter i used above has been defined independently of $x \in \not{k}$. However, for $x \notin \not{h}$, we know that $i = 0$ is indicated by the classical theory rather than the value defined above. Of course, if $\not{h}$ contains a Cartan subalgebra, then $D = E$ and hence the problem does not arise [as in the case of Spin (2,1) and Spin (2,2)]. Spin (4,2), however provides a counter example to this case.

(2) While for x regular and semisimple, $x \in \not{k}$, our results are fairly conclusive, we have not made any statements regarding the case when x is not regular. The condition x regular, however cannot be imposed *ab initio* in an extended Auslander–Kostant theory, for [e.g., in Spin (2,1) and Spin (2,2)] it is known that the supplementary series of representations cannot be derived using x regular. We hope to comment on these and related problems in a future communication.

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Geometric quantization and UIR's of semisimple Lie groups. III. Principal and supplementary series

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The principal and supplementary series representations of arbitrary semisimple Lie groups is analyzed in the framework of Auslander and Kostant's theory of UIR's of solvable Lie groups. As an illustration, we discuss a physically relevant symmetry group, Spin (4,2).

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I. INTRODUCTION

In a previous paper,[1] we have shown that the discrete series UIR's of G (G semisimple) arise in a natural manner from an extended Auslander–Kostant theory.[2] Here we discuss the case of the principal and supplementary series UIR's. Our major result is given by

Theorem: Let G be semisimple and let $\mathbf{h}$ be a θ-invariant split[3] Cartan subalgebra. Let $x\in\mathbf{h}\cap\mathbf{p}$ be quantizable. Let there exist a positive polarization, $\mathbf{s}_x$ at x. Let χ be the character on G_x associated with x. Let $S_x = G_x S_x^0$, where S_x^0 is the analytic subgroup of G^c with Lie algebra $\mathbf{s}_x$. Let χ' denote χ extended trivially to S_x. Then the following representations are equivalent.

(i) $\rho_1 = \mathrm{ind}_{E_c}^{G_c}(\overline{\mathrm{ind}}_{D_c}^{E_c}\chi)$,

(ii) $\rho_2 = \mathrm{ind}_{S_x}^{G_c}\chi'$,

where $\overline{\mathrm{ind}}$ denotes holomorphic induction and where D and E are defined as usual.

We prove this theorem in Sec. II. In Sec. III, we discuss a physically interesting symmetry group, Spin (4,2).

II. GENERAL THEORY AND PROOF OF THE THEOREM

Let G be semisimple and let $\mathbf{h}$ be a θ-invariant split Cartan subalgebra, i.e.,

$$\mathbf{h} = (\mathbf{h}\cap\mathbf{p}) \oplus (\mathbf{h}\cap\mathbf{k}), \tag{II.1}$$

$g = \mathbf{k} + \mathbf{p}$ being the Cartan decomposition.

Let Δ denote the set of roots relative to $(\mathbf{g},\mathbf{h})$. The following results are well known.

Proposition 1:

(i) If $\alpha\in\Delta$ is real on $\mathbf{h}$, then α vanishes on $\mathbf{h}\cap\mathbf{k}$.[4]

(ii) If $\alpha\in\Delta$ is pure imaginary on $\mathbf{h}$, then α vanishes[4] on $\mathbf{h}\cap\mathbf{p}$.

(iii) If α is complex, then $\bar{\mathbf{g}}_\alpha = \mathbf{g}_{\bar\alpha}$.

Let $x\in\mathbf{h}\cap\mathbf{p}$. Define

$$\langle\theta\rangle = \{\alpha\in\Delta : \alpha(x) = 0\}. \tag{II.2}$$

It is clear that

$$\mathbf{g}_x = \mathbf{h} + \mathbf{n}_1,$$

where

$$\mathbf{n}_1 = (\text{lin span}\{\mathbf{g}_\alpha : \alpha\in\langle\theta\rangle\})\cap\mathbf{g}. \tag{II.3}$$

Let Δ^+ be a positive subspace of Δ.

Proposition 2[5]: Let x be quantizable. There exists a positive polarization $\mathbf{s}_x$ at x which is of the form

$$\mathbf{s}_x = \mathbf{h} + \mathbf{n}_1 + \mathbf{n}_2,$$

where

$$\mathbf{n}_2 = \{\mathbf{g}_\alpha,\ \alpha\in\Delta^+,\ \alpha\notin\langle\theta\rangle\}. \tag{II.4}$$

for a suitable choice of Δ^+. Note, however, that $\mathbf{s}_x$ is not necessarily unique.

It is clear that

$$\delta = \mathbf{s}_x\cap\mathbf{g} = \mathbf{h} + \mathbf{n}_1 + (\mathbf{n}_2\cap\mathbf{g}),$$

$$e = (\mathbf{s}_x + \bar{\mathbf{s}}_x)\cap\mathbf{g} = \mathbf{h} + \mathbf{n}_1 + (\mathbf{n}_2 + \bar{\mathbf{n}}_2)\cap\mathbf{g}. \tag{II.5}$$

Lemma 1: Let χ be the character on G_x associated with x. Then χ is trivial on $\mathbf{s}_x/\mathbf{h}$.

Proof: This follows from the fact that the mapping $2\pi iB(x, -):\mathbf{g}_x\to i\mathbb{R}$, which is the differential of χ, is trivial on $\mathbf{g}_x/h$.

Consider the induction

$$\sigma_1 = \mathrm{ind}_{S_x}^{E_c}(\chi'). \tag{II.6}$$

The left covariance condition reads

$$\psi(gh) = \chi'(g)\psi(h),\quad g\in\mathbf{s}_x,\quad h\in E_c. \tag{II.7}$$

It is obvious that if $g\in D_c$, then Eq. (II.7) agrees with the corresponding condition for the induction

$$\sigma_2 = \overline{\mathrm{ind}}_{D_c}^{E_c}(\chi). \tag{II.8}$$

Assume accordingly that $g\in s_x/D_c$. One gets immediately, from Lemma 1,

$$\psi(gh) = \psi(h),\quad g\in s_x/D_c,\quad h\in E_c. \tag{II.9}$$

We take g of the form

$$g = \exp(\bar z'_\mu A_\mu),\quad A_\mu\in\mathbf{n}_2\quad \text{(no summation)}$$

and write h as

$$h = [\Pi\exp(\bar\xi_i A_i)\cdot\pi\exp(\eta_i\bar A_i)]\cdot h',\quad h'\in D_c,\ A_i\in\mathbf{n}_2,\ \bar A_i\in\bar{\mathbf{n}}_2. \tag{II.10}$$

On performing the multiplication, we get

$$gh = h''[\Pi\exp(\bar\xi'_i A_i)\cdot\pi\exp(\eta'_i\cdot\bar A_i)]\cdot h',\quad h''\in G_x/H. \tag{II.11}$$

Eq. (II.9) then becomes, using the fact that $\chi(h'') = 1$,

$$\psi[\Pi\exp(\bar\xi'_i\bar A_i)\cdot\Pi\exp(\eta'_i\cdot A_i)]\cdot h' = \psi[\Pi\exp(\xi_i A_i)\cdot\pi\exp(\eta_i\cdot\bar A_i)\cdot h']. \tag{II.12}$$

Differentiating the equation with respect to $\bar z'_\mu$, rewriting this differential in terms of $\partial\psi/\partial\bar\xi_\mu$, and putting $\bar z'_\mu = 0$, we find that

$$\partial\psi/\partial\bar\xi_\mu = 0, \tag{II.13}$$

which is just the holomorphicity condition. We have thus proved,

Lemma 2: Using notation as above,

$$\overline{\operatorname{ind}}{}_{D_c}^{E_c}(\chi) = \operatorname{ind}_{S_x}^{E_c}(\chi').$$

One immediately concluded that

$$\rho_1 = \operatorname{ind}_{E_c}^{G_c}(\overline{\operatorname{ind}}{}_{D_c}^{E_c}\chi) \approx \operatorname{ind}_{E_c}^{G_c}(\operatorname{ind}_{S_x}^{E_c}\chi') \approx \rho_2 \tag{II.14}$$

which proves the theorem stated in I.

III. APPLICATION TO SPIN (4,2)

We define the spin (4,2) Lie algebra by

$$[J_{ij}, J_{kl}] = g_{ik}J_{jl} + g_{jl}J_{ik} - g_{il}J_{jk} - g_{jk}J_{il},$$
$$J_{ij} = -J_{ji}, \quad i,j = 1,\ldots,6,$$

with

$$g_{ij} = \operatorname{diag}\{+1, +1, +1, +1, -1, -1\}. \tag{III.1}$$

We have,

$$\mathbf{k} = \{J_{12}, J_{13}, J_{14}, J_{23}, J_{24}, J_{34}, J_{56}\},$$
$$\mathbf{p} = \{J_{15}, J_{25}, J_{35}, J_{45}, J_{16}, J_{26}, J_{36}, J_{46}\}. \tag{III.2}$$

Let $\mathbf{h} = \{J_{15}, J_{26}, J_{34}\}$ with

$$\mathbf{h} \cap \mathbf{k} = \{J_{34}\}, \quad \mathbf{h} \cap \mathbf{p}\{J_{15}, J_{26}\}.$$

The roots are given by

$$\alpha_1 = (1, -1, 0), \quad \mathbf{g} \pm \alpha_1 = \{J_{12} \mp J_{25} \mp J_{56} \mp J_{16}\},$$
$$\alpha_2 = (0,1,i), \quad \mathbf{g} \pm \alpha_2 = \{J_{23} \mp J_{36} \pm i(J_{24} \mp J_{46})\},$$
$$\alpha_3 = (0,1,-i), \quad \mathbf{g} \pm \alpha_3 = \{J_{23} \mp J_{36} \mp i(J_{24} \mp J_{46})\},$$
$$\alpha_4 = (1,1,0), \quad \mathbf{g} \pm \alpha_4 = \{J_{12} \mp J_{25} + J_{16} \pm J_{56}\},$$
$$\alpha_5 = (1,0,i), \quad \mathbf{g} \pm \alpha_5 = \{J_{13} \mp J_{35} \pm i(J_{14} \mp J_{45})\},$$
$$\alpha_6 = (1,0,-i), \quad \mathbf{g} \pm \alpha_6 = \{J_{13} \mp J_{35} \mp i(J_{14} \mp J_{45})\}, \tag{III.3}$$

where, i.e., $\alpha_1 = (1, -1, 0)$ means that

$$\alpha_1(J_{15}) = -\alpha_1(J_{26}) = 1, \quad \alpha_1(J_{34}) = 0.$$

Let $x = b_1J_{15} + b_2J_{26}$, $b_1, b_2 \in \mathbb{R}$. We have the following classes of orbits:

(i) $b_1, b_2 \neq 0$, $|b_1| \neq |b_2|$, $\mathbf{g}_x = \mathbf{h}$,

(ii) $b_1 = b_2 \neq 0$, $\mathbf{g}_x = \mathbf{h} + \mathbf{g}_{\alpha_1} + g_{-\alpha_1}$,

(iii) $b_1 = -b_2 \neq 0$ $\mathbf{g}_x = \mathbf{h} + \mathbf{g}_{\alpha_4} + \mathbf{g}_{-\alpha_4}$,

(iv) $b_1 = 0, b_2 \neq 0$,

$$\mathbf{g}_x = \mathbf{h} + (\mathbf{g}_{\alpha_5} + \mathbf{g}_{-\alpha_5} + \mathbf{g}_{\alpha_6} + \mathbf{g}_{-\alpha_6}) \cap \mathbf{g},$$

(v) $b_1 \neq 0, b_2 = 0$,

$$\mathbf{g}_x = \mathbf{h} + (\mathbf{g}_{\alpha_2} + \mathbf{g}_{-\alpha_2} + \mathbf{g}_{\alpha_3} + \mathbf{g}_{-\alpha_3}) \cap \mathbf{g}. \tag{III.4}$$

In all the cases, X is quantizable. The corresponding positive polarizations are given by

$$\mathbf{s}_x = \mathbf{g}_x + \mathbf{s}'_x,$$

where $\mathbf{s}'_x$ could be any of the 24 subalgebras listed in Table I. Here, a $\pm$ sign under i, $i = 1,\ldots,6$, indicates $\mathbf{g}_{\pm\alpha_i} \subseteq \mathbf{s}'_x$ respectively. Further, χ is trivial on $\mathbf{g}_x / \{J_{15}, J_{26}\}$. The corresponding representations of G thus form a subset of the set of principal and supplimentary series defined by Harish Chandra.[6]

TABLE I. Forms of $\mathbf{s}_x$ [Eq. (III.5)]. A $\pm$ sign under i, $i = 1,\ldots,6$ implies $\mathbf{g}_{\pm\alpha_i} \subseteq \mathbf{s}'_x$ resp.

S. No.	1	2	3	4	5	6
1	+	+	+	+	+	+
2	+	+	−	+	+	+
3	+	+	−	+	+	−
4	+	+	−	−	+	−
5	+	−	+	+	+	+
6	+	−	+	−	−	+
7	+	−	+	−	−	+
8	+	−	−	+	+	+
9	+	−	−	+	+	+
10	+	−	−	+	+	−
11	+	−	−	−	−	+
12	+	−	−	−	−	−
13	−	+	+	+	+	+
14	−	+	+	+	+	−
15	−	+	+	−	−	+
16	−	+	+	−	−	−
17	−	+	+	−	−	−
18	−	+	−	+	+	−
19	−	+	−	+	+	−
20	−	+	−	−	−	−
21	−	−	+	−	−	+
22	−	−	+	−	−	+
23	−	−	+	−	−	−
24	−	−	−	−	−	−

IV. CONCLUSIONS

We have succeeded in reproducing some of the representations defined by Harish Chandra *et al.* using the Auslander–Kostant induction scheme. One may possibly hope to rederive all the known principal and supplementary series representations by using a modified induction scheme,

$$\sigma' = \operatorname{ind}_{E_c}^{G_c}(\overline{\operatorname{ind}}{}_{D_c}^{E_c}\sigma),$$

where σ is an arbitrary UIR of D_c. However, the relationship between σ and the point $x \in \mathbf{g}$ under consideration (as exists if σ is a character) is not yet transparent. An analogous situation arises if we choose σ to be nonunitary representation in order to rederive the complementary series of representations.

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Anomalies and eigenvalues of Casimir operators for Lie groups and supergroups [a)]

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An expression for the anomaly of any representation of the SU(N) groups and SU(N/M) supergroups is presented. Some anomaly free complex representations of SU(N) and SU(N/M) are pointed out. For SU(N) these occur for $N \geqslant 5$ and for large dimensions. For SU(N/M) they already occur for low dimensions. Also a generating function to obtain the eigenvalues of all Casimir operators of SU(N/M) is given and an extension to other supergroups is pointed out.

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To construct a renormalizable nonabelian gauge theory, one should avoid triangle anomalies.[1] Also in a gauge theory with zero mass fermionic bound states, in addition to elementary fermions, anomalies calculated in terms of elementary or composite fermions should be the same for consistency. 't Hooft suggested[2] to use this as a constraint to search for possible models with a zero mass fermion spectrum. He[2] and other authors[3–5] found various solutions. In particular, the supergroup SU(N/M) has been used as a tool to investigate 't Hooft constraints.[3,4] It is desirable to have an expression for the anomalies of various representations of supergroups to facilitate further investigations. A formula to calculate the anomaly of a general representation of SU(N) is given in the literature.[6,7,16] In this paper we give the anomaly of any representation of SU(N) in Young tableau parametrization and extend this result to the SU(N/M) case. The anomaly is proportional to the eigenvalue of the cubic Casimir operator.[7] One can calculate higher order Casimir invariants in the same way.[8] We conclude this paper by describing a procedure to obtain the eigenvalues of higher order Casimir operators of supergroups starting from the expressions for SU(N) and O(N) given in the literature.[9,10]

The anomaly of the representation R,$A(R)$, is given by[6]

$$\tfrac{1}{2}A(R)d_{abc} = \mathrm{Tr}[\{R(Q_a),R(Q_b)\}R(Q_c)], \tag{1}$$

where the matrices $R(Q_a)$ are the generators of the gauge group in the representation R. For the group SU(N), the d symbol, which is completely symmetric, is defined by the relation

$$\{\lambda_a,\lambda_b\} = (4/N)\delta_{ab}I_N + 2d_{abc}\lambda^c, \tag{2}$$

where I_N is the $N\times N$ unit matrix and $\lambda_a/2$ are the generators in the fundamental representation. Note that there is a factor of 2 between this normalization and that of ref. 6. We take λ_a's to be traceless and normalize them according to $\mathrm{Tr}(\lambda_a\lambda_b) = 2\delta_{ab}$. We define the third order Casimir operator $C_3(R)$ in the representation R as

$$C_3(R) = d_{abc}R(Q^a)R(Q^b)R(Q^c). \tag{3}$$

Using Eqs. (2) and (3), and the fact that the Casimir operator is proportional to unity, Eq. (1) can be rewritten as

$$A(R) = \frac{C_3(R)}{C_3(1)}\frac{\mathrm{Tr}_R(I)}{\mathrm{Tr}_1(I)}. \tag{4}$$

In this expression $\mathrm{Tr}_R(I)$ and $\mathrm{Tr}_1(I)$ are the traces of the identity element of the group for the representation R and the fundamental representation, respectively. $C_3(1)$ is the Casimir operator in the fundamental representation. For Lie groups, in particular for SU(N), the trace of identity is equal to the dimension of the representation considered.

A method to obtain eigenvalues of any Casimir invariant starting from the characters is given in Ref. 8. We describe it here for completeness. We denote a given representation of SU(N) by $(n_1,n_2,\ldots,n_{N-1},0)$, where n_i is the number of the boxes in the i'th row of the corresponding Young tableau. The character $\chi_{(n_1,n_2,\ldots)}$ of this representation is[8,11]

$$\chi_{(n_1,n_2,\ldots,n_{N-1})} = \det(h_{n_i-i+j}), \tag{5}$$

where we have shown the (ij)th element of the matrix, the determinant of which is calculated. h_m in the above expression is the character of the representation $(m,0,0,\ldots,0)$ corresponding to the tableau with a single row of m boxes and is given by[8]

$$h_m = \oint\frac{dz}{2\pi i}\frac{z^{-n-1}}{\det(1-zU)}, \tag{6}$$

where U is the group element in the fundamental representation $(1,0,0,\ldots,0)$. Since any group element can be written in the form $g = \exp(\alpha^a Q_a)$ we can write the $C_3(R)$ as[8]

$$C_3(R) = d_{abc}\left|\frac{\partial^3}{\partial\alpha_a\partial\alpha_b\partial\alpha_c}R(g)\right|_{\alpha=0}, \tag{7}$$

where $R(g)$ is the representation of g. Upon taking the traces of both sides we find

$$d(R)C_3(R) = d_{abc}\left|\frac{\partial^3}{\partial\alpha_a\partial\alpha_b\partial\alpha_c}\chi_R(g)\right|_{\alpha=0}. \tag{8}$$

We first calculate $C_3(m)$, the eigenvalue of the Casimir operator in the completely symmetric representation $(m,0,0,\ldots,0)$. Using Eqs. (6) and (8) we find

$$C_3(m) = C_3(1)\frac{m(N+m)(N+2m)}{(N+2)(N+1)}. \tag{9}$$

Upon substituting Eq. (9) into Eq. (4) we get

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$$\frac{A(m)}{d_m} = \frac{m(N+m)(N+2m)}{N(N+1)(N+2)} A_1, \tag{10}$$

$$d_m = \frac{1}{m!} N(N+1)(N+2)\dots(N+m-1) = h_m(1),$$

where $A(m)$ and d_m are the anomaly and the dimension of the representation (m,0,...,0). Assuming $A_1 \neq 0$ [which is true except for SU(2)] we may normalize it to $A_1 = 1$. This result agrees with Ref. 6. Similarly differentiating Eq. (5) we obtain the anomaly $A(n_1,n_2,\dots,n_l,0,\dots)$ of the representation $(n_1,n_2,\dots,n_l,0,\dots)$ as[8]

$$A(n_1,n_2,\dots,n_l,0,\dots) = \begin{vmatrix} A(n_1) & d_{n_2-1} & d_{n_3-2} & \cdot & \cdot & \cdot \\ A(n_1+1) & d_{n_2} & d_{n_3-1} & \cdot & \cdot & \cdot \\ A(n_1+2) & d_{n_2+1} & d_{n_3} & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} + \begin{vmatrix} d_{n_1} & A(n_2-1) & d_{n_3-2} & \cdot & \cdot & \cdot \\ d_{n_1+1} & A(n_2) & d_{n_3-1} & \cdot & \cdot & \cdot \\ d_{n_1+2} & A(n_2+1) & d_{n_3} & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} + \begin{vmatrix} d_{n_1} & d_{n_2-1} & A(n_3-2) & \cdot & \cdot & \cdot \\ d_{n_1+1} & d_{n_2} & A(n_3-1) & \cdot & \cdot & \cdot \\ d_{n_1+2} & d_{n_2+1} & A(n_3) & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} + \cdots, \tag{11}$$

where the dimension of each determinant is equal to l, the number of rows in the Young tableau. In the above expression the number of determinants in the sum is also l. This agrees with the previous results which are given in different forms.[6,9]

One can use the formula for the eigenvalues of the cubic Casimir operator given in Ref. 9 to write down a concise expression for the anomaly. We give the result in two identical forms. One of these is

$$\frac{A(n_1,n_2,\dots,n_l,0,\dots,0)}{d(n_1,n_2,\dots,n_l,0,\dots,0)} = \frac{N}{(N^2-1)(N^2-4)} \Big[2\sum_{i=1}^{l} n_i^3 + 3b \sum_{i=1}^{l} (n_i^2 - 2in_i) + 6\sum_{i=1}^{l} (i^2 n_i - in_i^2) + n(b^2+b-2n) \Big], \tag{12}$$

where n is the total number of boxes in the Young tableau,

$$n = n_1 + n_2 + \cdots + n_l, \tag{13a}$$

and

$$b = N + 1 - 2n/N. \tag{13b}$$

Equation (12) can be recast into yet another form:

$$\frac{A(n_1,n_2,\dots)}{d(n_1,n_2,\dots)} = \frac{2N}{(N^2-1)(N^2-4)} \sum_{i=1}^{N} \left(n_i - i - \frac{n}{N} + \frac{N+1}{2} \right)^3. \tag{14}$$

For possible applications in grand unified theories and theories of composite quarks and leptons[2–5] it is of interest to inquire whether there are anomaly-free, complex, irreducible representations of SU(N) type groups. Using Eq. (12) we calculated the anomaly of the representations of the groups SU(N),$4 \leqslant N \leqslant 9$, with dimension less than 1000. We found that the only anomaly-free representations among these are the real representations. However, for large values of n there are anomaly-free, complex, irreducible representations of SU(N),$N \geqslant 5$. We give some examples of anomaly-free, complex, irrreducible representations of SU(N) groups in Table I.

We denote the generators of the supergroup SU(N/M) by $X_A, A = a,\alpha$. These form a superalgebra. $X_a, a = 1,\dots,N^2+M^2-1$ are the even elements and $X_\alpha, \alpha = 1,\dots,2NM$ are the odd elements of the superalgebra. The grade of the index A is defined as $g(a) = 0, g(\alpha) = 1$. For the supergroup SU(N/M) we again define the d symbol by the relation.

TABLE I. Some anomaly-free, *complex*, irreducible representations of SU(N) groups, in Young tableau parametrization.

N	Representation
	(13,13,6,3,0)
5	(13,10,7,0,0)
	(12,9,6,6,0,0)
6	(12,12,6,6,3,0)
	(11,8,6,6,4,0,0)
	(11,8,7,6,3,0,0)
	(11,8,8,6,2,0,0)
	(11,9,9,6,0,0,0)
7	(11,11,7,5,5,3,0)
	(11,11,8,5,4,3,0)
	(11,11,9,5,3,3,0)
	(11,11,11,5,2,2,0)
	(10,7,5,5,5,4,0,0)
	(10,7,6,5,5,3,0,0)
	(10,7,7,5,5,2,0,0)
	(10,8,8,5,5,0,0,0)
8	(10,10,6,5,5,5,3,0)
	(10,10,7,5,5,4,3,0)
	(10,10,8,5,5,3,3,0)
	(10,10,10,5,5,2,2,0)
	(9,6,5,5,5,3,3,0,0)
	(9,6,6,5,5,3,2,0,0)
	(9,6,6,6,5,2,2,0,0)
	(9,7,7,5,5,3,0,0,0)
	(9,7,7,6,5,2,0,0,0)
9	(9,7,7,7,5,1,0,0,0)
	(9,9,6,6,4,4,4,3,0)
	(9,9,7,6,4,4,3,3,0)
	(9,9,7,7,4,3,3,3,0)
	(9,9,9,6,4,4,2,2,0)
	(9,9,9,7,4,3,2,2,0)
	(9,9,9,8,4,2,2,2,0)
	(8,5,4,4,4,4,3,3,0,0)
	(8,5,5,4,4,4,3,2,0,0)
	(8,5,5,5,4,4,2,2,0,0)
	(8,6,6,4,4,4,3,0,0,0)
	(8,6,6,5,4,4,2,0,0,0)
	(8,6,6,6,4,4,1,0,0,0)
10	(8,8,5,5,4,4,4,4,3,0)
	(8,8,6,5,4,4,4,3,3,0)
	(8,8,6,6,4,4,3,3,3,0)
	(8,8,8,5,4,4,4,2,2,0)
	(8,8,8,6,4,4,3,2,2,0)
	(8,8,8,7,4,4,2,2,2,0)

$$\{\lambda_A, \lambda_B\} = \frac{4}{\eta(N-M)} g_{AB} I_{N+M} + 2 d_{ABC} \lambda_C, \qquad (15)$$

where the $(N+M)\times(N+M)$ supertraceless matrices $\lambda_A/2$ are the generators in the fundamental representation, $\eta = +1(-1)$ for the class I (II) representations. The metric g_{AB} is not symmetric and related to the normalization of λ matrices by a supertrace[8]:

$$\mathrm{Str}(\lambda_A \lambda_B) = 2 g_{AB} \qquad (16)$$

with $g_{AB} = (-1)^{g(A)\cdot g(B)} g_{BA}$. We note that d_{ABC} as defined by Eq. (15) is symmetric for even indices, but antisymmetric for odd indices. We define the third order Casimir operator analogously to Eq. (3), except for using the d symbol of the supergroup SU(N/M).

For supergroups the anomaly of a representation R, $A(R)$, takes the form

$$\tfrac{1}{2} A(R) d_{ABC} = \mathrm{Str}[\{\mathrm{R}(\mathrm{X_A}), \mathrm{R}(\mathrm{X_B})\} \mathrm{R}(\mathrm{X_C})]. \qquad (17)$$

For supergroups Casimir operators are proportional to unity only for the representations where the dimension of the bosonic supspace is *not* equal to the dimension of the fermionic subspace[17]. For such representations Eq. (17) can be written in an analogous form to Eq. (4):

$$A(R) = \frac{C_3^{N,M}(R)}{C_3^{N,M}(1)} \frac{\chi_R(I)}{\chi_1(I)}, \qquad (18)$$

where C_3's are eigenvalues of the Casimir operators for the representation R and the fundamental representation and χ's are the characters of identity for these representations. Note that for supergroups, the character is defined as the supertrace of the matrix representation.[8]

A detailed study of the representations of supergroups is given in Refs. 8 and 12. In this paper we will examine class I representations only. Generalization of our results to class II representations is straightforward.

We first consider class I representations constructed from only covariant bases. We denote a given class I covariant representation of SU(N/M)) by $(n_1, n_2, \ldots)$, where n_i is the number of boxes at the i'th row of the corresponding supertableau.[8] The character of this representation is[8]

$$\chi_{(n_1, n_2, \ldots)} = \det(H_{n_i - i + j}), \qquad (19)$$

where H_m, the character of the representation $(m,0,0,\ldots)$, is

$$H_m = \oint \frac{dz}{2\pi i} \frac{z^{-n-1}}{\mathrm{Sdet}(1 - z\mathscr{U})}, \qquad (20)$$

with $\mathscr{U}$ being the supergroup element in the fundamental representation. Following the methods of Ref. 8 we can obtain the eigenvalue of the third order Casimir operator for the supergroup SU(N/M) as

$$\chi(I) C_3^{N,M}(R) = d_{ABC} \left[\frac{\partial^3}{\partial \alpha_A \partial \alpha_B \partial \alpha_C} \chi_R(g) \right]_{\alpha = 0}. \qquad (21)$$

Equations (20) and (21) give $C_3(m)$, the eigenvalue of the Camir operator for the representation corresponding to the supertableau with a single row of m boxes, as

$$C_3^{N,M}(m) = C_3^{N,M}(1) \frac{m(N-M+m)(N-M+2m)}{(N-M+2)(N-M+1)}, \qquad (22)$$

which agrees with Ref. 4. Equations (18) and (22) yield

$$\frac{A(m)}{\chi_m(I)} = \frac{m(N-M+m)(N-M+2m)}{(N-M)(N-M+2)(N-M+1)}, \qquad (23)$$

$$\chi_m(I) = \frac{1}{m!}(N-M)(N-M+1)\cdots(N-M+m-1) = H_m(I),$$

where $\chi_m(I)$ is the character of identity (which is equal to the number of bosons *minus* the number of fermions) and $A(m)$ is the anomaly for the representation $(m,0,0,\ldots)$. Similarly differentiating Eq. (19) we find the anomaly $A(n_1, n_2, \ldots, n_l, 0, \ldots)$ of the covariant class I representation $(n_1, n_2, \ldots, n_l, 0, \ldots)$ as

$$A(n_1, n_2, \ldots, n_l, 0 \ldots) = \begin{vmatrix} A(n_1) & \chi_{n_2 - 1}(I) & \cdot & \cdot & \cdot \\ A(n_1+1) & \chi_{n_2}(I) & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} + \begin{vmatrix} \chi_{n_1}(I) & A(n_2 - 1) & \cdot & \cdot & \cdot \\ \chi_{n_1+1} & A(n_2) & \cdot & \cdot & \cdot \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{vmatrix} + \cdots. \qquad (24)$$

Now, if we compare this expression for SU(N/M) to Eq. (11) for SU(N), we note that they are formally the same except for the replacement of N by N-M. Indeed this observation[13] is true for all Casimir operators as can be derived from the expressions in Ref. 8. Therefore we can simplify our expression and obtain a result similar to Eq. (12) in terms of sums of powers of n_i. We find that

$$\frac{A(n_1, n_2, \ldots n_l, 0, \ldots)}{\chi_{(n_1, n_2, \ldots n_l, 0, \ldots)}(I)} = \frac{(N-M)}{[(N-M)^2 - 1][(N-M)^2 - 4]} \times \left[2 \sum_{i=1}^{l} n_i^3 + 3\beta \sum_{i=1}^{l} (n_i^2 - 2i n_i) + 6 \sum_{i=1}^{l} (i^2 n_i - i n_i^2) + n(\beta^2 + \beta - 2n) \right], \qquad (25)$$

where again $n = n_1 + \cdots + n_l$ and $\beta = N - M + 1 - [2n/(N-M)]$. Using Eq. (25) one can find a number of anomaly-free representations of SU(N/M). In particular, class I representations of the supergroup SU($N + r/N$) corresponding to the supertableaux with the same shape as those of the *real* representations of SU(r) (with $r > 3$) are anomaly-free. From Ref. 8 it can be seen that the same result applies to the class II representations of the supergroup SU($N/N + r$) which have supertableaux reflected from the diagonal relative to those of SU($N + r/N$). These are complex representations of the supergroups and were used in Ref. 3 with $r = 4$ for the representation $(2,0,\ldots)$ to construct a model of composite quarks and leptons that satisfy the anomaly constraints of 't Hooft.

Character formulas for the class I (and also class II) representations constructed from only contravariant as well as mixed (covariant *and* contravariant) basis vectors is given in Ref. 8. Using those expressions and Eq. (21) one can obtain

obtain anomaly expressions in determinantal forms similar to Eq. (24). In particular we have the relation

$$A(\ldots,-n_3,-n_2,-n_1;0,0,\ldots)=-A(\ldots,0,0;n_1,n_2,n_3,\ldots) \quad (26)$$

between the anomalies of the covariant representation $(\ldots,0,0;n_1,n_2,n_3,\ldots)$ and the contravariant representation $(\ldots,-n_3,-n_2,-n_1;0,0,\ldots)$.

With the recent advent of dynamical supersymmetries in nuclear physics[14] one particularly needs the eigenvalues of linear and quadratic Casimir operators. Reference 8 gives an expression for the eigenvalues of any Casimir operator. However, the determinantal forms of Ref. 8 can be simplified using the methods of Ref. 9. We only need to note that $SU(N/M)$ Casimir eigenvalues can be obtained from the corresponding $SU(N)$ eigenvalues by replacing N by N-M, as follows from the expressions in Ref. 8, and as illustrated above for the cubic Casimir operator.

The standard definition of the pth order Casimir operator of $SU(N/M)$ is[15]

$$C_p^{N,M}=T_{i_2}{}^{i_1}T_{i_3}{}^{i_2}\cdots T_{i_1}{}^{i_p}(-1)^{g(i_2)+g(i_3)+\cdots+g(i_p)}, \quad (27a)$$

where the generators $T_i{}^j$ are related to the previously defined generators X_A via the relation

$$\tfrac{1}{2}T_i{}^j(\lambda_A)_j{}^i=X_A. \quad (27b)$$

Note that a cubic Casimir operator defined in this way differs from our previous definition [Eq. (3)], which is more suitable for anomaly considerations, by quadratic Casimir operator. We give the result for covariant representations of $SU(N/M)$. C_0 is defined to be $N-M$. The generating function for the Casimir operators of $SU(N/M)$ is

$$\sum_{p=0}^{\infty}C_p^{N,M}z^p = (N-M)\exp[-f(z)]+\{1-\exp[-f(z)]\}z^{-1}, \quad (28)$$

where

$$f(z)=\sum_{k=2}^{\infty}b_kz^k \quad \text{with } b_k=\frac{1}{k}\sum_{j=1}^{k-1}\binom{k}{j}S_j. \quad (29)$$

For the covariant class I representation $(n_1,n_2,\ldots,n_l,0,\ldots)$, with $l<N-M$, S_j is given as

$$S_j=\sum_{i=1}^{N-M}\sum_{t=0}^{j-1}\binom{j}{t}\left(n_i-\frac{n}{N-M}\right)^{j-t}(N-M-i)^t, \quad (30)$$

where n is the total number of boxes in the supertableau. We again emphasize that the above expressions are valid only for the representations where the dimension of fermionic subspace is different from the dimension of bosonic subspace. Using Eqs. (27)–(29) we can write the eigenvalues of the quadratic Casimir invariant for the representation $(n_1,n_2,\ldots,n_l,0,\ldots)$ of $SU(N/M)$:

$$C_2^{N,M}=\frac{1}{2}\left\{\sum_{i=1}^{l}(n_i^2-2in_i)+(N-M+1)n-\frac{n^2}{N-M}\right\}. \quad (31)$$

One can similarly obtain the Casimir invariants of the supergroup $OSP(N/2M)$ from the expressions for $O(N)$ given in Ref. 10 by substituting $N-2M$ in place of N.

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Dimensions of orbits and strata in complex and real classical Lie algebras [a]

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Explicit expressions for codimensions of orbits and strata of elements of complex Lie algebras $gl(n, \mathbb{C})$, $o(n, \mathbb{C})$, $sp(2n, \mathbb{C})$ and real Lie algebras $gl(n, \mathbb{R})$, $gl(n, \mathbb{H})$, $u(p, q)$, $o(p, q)$, $o^*(2n)$, $sp(2n, \mathbb{R})$, and $sp(2p, 2q)$ are given. They make it possible to list easily all dimensions of orbits and strata in a given Lie algebra. The dimension of an orbit or stratum of a given matrix, an element of one of the Lie algebras in its natural representation, can be determined from our formulas after the matrix has been transformed into its Jordan normal form in $gl(n, \mathbb{C})$, $gl(n, \mathbb{R})$, or $gl(n, \mathbb{H})$. Stratification of the Lie algebra in the vicinity of a singular element is discussed.

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1. INTRODUCTION

It is generally accepted that fundamental physical interactions are determined by a spontaneously broken gauge symmetry.[1–3] The symmetry is characterized by the fact that an interaction potential (Higgs potential) has a minimum on a nontrivial group orbit. Therefore the orbit structure of representations of some compact semisimple Lie algebras has been needed often and a number of particular cases were studied in detail (cf. Refs. 1–3 and references therein). Orbits and strata of representations of noncompact semisimple Lie algebras are equally of interest; their structure is richer. One of the representations invariably appearing in particle physics is the adjoint one. In this case one often speaks of conjugacy classes of elements of the Lie algebra because they coincide with the orbits.

In mathematics also much attention has been devoted to conjugacy classes of elements (cf. Ref. 4 and references therein). It is curious to notice that the orbits of interest in elementary particle physics are the critical orbits which are of smallest dimension, while in mathematics those which are best studied are the largest, called regular and subregular orbits.[4,5]

In this article we consider two related stratifications of real and complex classical Lie algebras: (i) into orbits under the action of the corresponding Lie group, and (ii) into families of orbits, called strata, containing elements of the same structure, i.e., having conjugate centralizers under the action of the corresponding group.

Consider first an example, the Lie algebra $gl(2, \mathbb{C}) \simeq \mathbb{C}^{2\times 2}$. It is a union of three strata of 2×2 complex matrices:

1. Matrices with distinct eigenvalues; they form an open dense set of $\mathbb{C}^{2\times 2}$.

2. Matrices similar to a 2×2 Jordan block; these form a semialgebraic (i.e., defined by equalities and inequalities) submanifold of codimension one.

3. Multiples of the identity matrix (scalar matrices); this is an algebraic submanifold of codimension three in $gl(2, \mathbb{C})$.

Clearly orbits belonging to the same stratum are distinguished by the eigenvalues. In the first and the second case the orbits have dimension two; in the third an orbit is just a point. The union of strata *2* and *3* is an algebraic subvariety of $\mathbb{C}^{2\times 2}$ isomorphic to the direct product of a cone and a line, and the set of the scalar matrices is the direct product of the vertex of the cone with the line.

The purpose of this paper is to answer the following two questions about the dimensions of orbits and strata in complex and real classical Lie algebras: 1. What are the dimensions occurring in a given Lie algebra? 2. Given a matrix, an element of a given Lie algebra, what is the dimension of its orbit or stratum?

It turns out that the dimension of the orbit and stratum of a matrix depends only on its Jordan normal form in $gl(N, \mathbb{C})$, $gl(N, \mathbb{R})$, or $gl(N, \mathbb{H})$ according to the case, and not on the additional Lie-algebra structure.

In what follows elements of a Lie algebra (group) are identified with their natural matrix representations. It is advantageous to consider codimensions d of the orbits and codimensions c of the strata rather than the respective dimensions D and C. Obviously,

$$D = N - d, \quad C = N - c, \quad d \geqslant c, \tag{1}$$

where N is the dimension of the Lie algebra. Together with the codimensions of orbits we present the codimensions of strata. Strata with codimension $c > 0$ are called singularities. In general, strata are semialgebraic submanifolds.

The results for $gl(n, \mathbb{C})$ and $gl(n, \mathbb{R})$ are in Ref. 6. They are also in Refs. 7 and 8, respectively, and these techniques are generalized to the other cases. The dimension formulas of Ref. 9 for $sp(2n, \mathbb{R})$ are simplified here. For $o(n, \mathbb{C})$ and $sp(2n, \mathbb{C})$ they are in Ref. 10. The remaining cases are new here.

Our expressions for the codimensions d of orbits were obtained by direct computation of the centralizers of representatives of conjugacy classes of elements.[11,12] Another way to arrive at the same results would be to use the description of the centralizers given in Ref. 4. Since each stratum contains orbits of the same codimension d, the codimension c of a stratum is obtained from d by subtracting from it the num-

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ber of distinct nonzero real (complex) numbers necessary to specify the eigenvalues of a generic element of the stratum of a real (complex) Lie algebra. However, c can be computed from any element of the stratum.

Section 2 contains explicit formulas for the codimensions d and c of all orbits and strata in all complex and real classical Lie algebras. In Sec. 3 a local stratification of a Lie algebra is described in the neighborhood of an element belonging to a stratum of small codimension. Section 4 contains some remarks and conclusions.

2. CODIMENSIONS OF ORBITS AND STRATA

Here we first introduce some conventions and then give explicit formulas for d and c.

We denote the Lie algebras as in Ref. 13. In our computations the normal forms of representatives of conjugacy classes were used.[11,12] A conjugacy class is represented by a direct sum of generalized Jordan blocks

$$\begin{pmatrix} a & I & & & \\ & \cdot & \cdot & & \\ & & \cdot & \cdot & \\ & & & \cdot & I \\ & & & & a \end{pmatrix} \tag{2}$$

and their transposed with entries either numbers (in $\mathbb{R}$,$\mathbb{C}$,$\mathbb{H}$) or 2×2 matrices. However, one does not need to be familiar with details of Refs. 11 or 12 in order to find the dimension of the orbit to which a matrix (an element of a given Lie algebra) belongs. Indeed, it suffices to bring the matrix to its Jordan normal form [in $gl(n, \mathbb{C})$ or $gl(n, \mathbb{R})$ or $gl(n, \mathbb{H})$ according to the case] ignoring the details of its Lie algebra structure, and to use the information about its structure and eigenvalues in the formulas below. The Jordan form in $gl(n, \mathbb{R})$ and $gl(n, \mathbb{H})$ consists of the generalized blocks of type (2) associated with pairs of eigenvalues $a \pm ib$. The actual computation of these formulas was lengthy but straightforward. We present just the results, a few comments, and examples.

Algebra $gl(n, \mathbb{C})$

If an element has distinct eigenvalues $\alpha_1,...,\alpha_r$, each corresponding to a direct sum of Jordan blocks of respective orders $n_1^i \geqslant n_2^i \geqslant \cdots \geqslant n_{v_i}^i$, then

$$d = \sum_{i=1}^{r} \sum_{j=1}^{v_i} (2j-1) n_j^i, \tag{3}$$

$$c = d - r. \tag{4}$$

Algebra $gl(n, \mathbb{R})$

Formula (3) applies in this case with any pair of complex conjugate eigenvalues $a \pm ib$ counted as one α_j. The Jordan blocks are now real. Also

$$c = d - \nu, \tag{5}$$

where ν denotes the number of distinct eigenvalues.

Algebra $gl(n, \mathbb{H})$

If an element has pairs of complex conjugate eigenvalues $(\alpha_1, \alpha_1^*),...,(\alpha_r, \alpha_r^*)$ corresponding Jordan blocks with entries which are 2×2 complex matrices $\left(\begin{smallmatrix} \gamma & \beta \\ -\beta^* & \gamma^* \end{smallmatrix}\right)$ (representing quaternions) and of respective orders $n_1^i \geqslant n_2^i \geqslant \cdots \geqslant n_{v_i}^i$, and real eigenvalues $a_1,...,a_s$ corresponding to Jordan blocks of respective orders $m_1^i \geqslant \cdots \geqslant m_{u_i}^i$, then

$$d = \sum_{i=1}^{r} \sum_{j=1}^{v_i} (2j-1) n_j^i + 2 \sum_{i=1}^{s} \sum_{j=1}^{u_i} (2j-1) m_j^i, \tag{6}$$

$$c = d - \nu, \tag{7}$$

where ν is the number of distinct eigenvalues.

Algebras $o(n, \mathbb{C})$ and $sp(2n, \mathbb{C})$

If an element has nonzero eigenvalues $\alpha_1,...,\alpha_r$, each α_i corresponding to Jordan blocks of respective orders $n_1^i \geqslant \cdots \geqslant n_{v_i}^i$, and Jordan blocks of orders $N_1 \geqslant \cdots \geqslant N_s$ of zero eigenvalues, t of these blocks being of odd order, then

$$d = \frac{1}{2} \left(\sum_{i=1}^{r} \sum_{j=1}^{v_i} (2j-1) n_j^i + \sum_{k=1}^{s} (2k-1) N_k - \epsilon t \right), \tag{8}$$

where $\epsilon = +1$ for $o(n, \mathbb{C})$ and $\epsilon = -1$ for $sp(2n, \mathbb{C})$

$$c = d - \frac{r}{2} - \delta, \tag{9}$$

with

$$\delta = \begin{cases} 1 & \text{if 0 is an eigenvalue of multiplicity 2 and } \epsilon = 1, \\ 0 & \text{otherwise.} \end{cases} \tag{10}$$

Note that d is half of (3) minus $\frac{1}{2}\epsilon t$.

Algebras $o(p, q)$ $(\epsilon = +1)$ and $sp(2n, \mathbb{R})$ $(\epsilon = -1)$

Codimension d is given by (8) where pairs of complex conjugate eigenvalues $a \pm ib$ are counted as one α_j. The Jordan blocks are real.

$$c = d - \tfrac{1}{2}\nu - \delta, \tag{11}$$

where ν is the number of nonzero eigenvalues and δ is given by (10).

Algebras $sp(2p, 2q)$ and $o^*(2n)$

The dimension d is equal to half of (6)

$$c = d - \tfrac{1}{2}\nu - \delta', \tag{12}$$

where ν is the number of nonzero eigenvalues and

$$\delta' = \begin{cases} 1 & \text{if 0 is an eigenvalue of multiplicity 2 and } \epsilon = -1 \\ 0 & \text{otherwise.} \end{cases}$$

Algebra $u(p, q)$

In this case the dimensions d and c are given by (3) and (4), respectively.

Let us point out that a stratum of elements of a given Lie algebra contains all matrices with the same structure of Jordan blocks corresponding to eigenvalues of the same type.

It follows from computing the centralizers that the notion of the stratum of elements of a Lie algebra and the notion of "the set of elements of the Lie algebra having the same Jordan normal form" are closely related. Namely one has the following

1. The two notions coincide for $gl(n, \mathbb{C})$, $gl(n, \mathbb{R})$, $gl(n, \mathbb{H})$, $sp(2n, \mathbb{C})$, and $sp(2n, \mathbb{R})$.

2. Elements of the orthogonal algebras $o(n, \mathbb{C})$, $o(p, q)$, and $o^*(2n)$ with the eigenvalue zero of multiplicity 2 belong to strata which contain also elements of another Jordan normal form (see examples below).

3. For the algebras $o(p, q)$, $u(p, q)$, [resp. $sp(2p, 2q)$] a Jordan normal form of an element can be divided into two parts of order p and q (resp. $2p$ and $2q$) according to the signature of the algebra. A stratum contains only elements with the same Jordan normal forms within each of the two parts.

For example, the matrices $\begin{pmatrix} \beta & 0 \\ 0 & -\beta \end{pmatrix}$ with $\beta \neq 0$ and $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$ belong to the same stratum in $o(2, \mathbb{C})$ but to different strata in $sl(2, \mathbb{C})$; in the first case their centralizers coincide, in the second one they are different. In general, whenever matrices with different Jordan normal forms belong to the same stratum, the one with the eigenvalue 0 of multiplicity 2 is a special case of the other.

Consider the matrix

$$M_1 = M(b, b') = \begin{pmatrix} 0 & b & 1 & & & & & \\ -b & 0 & & 1 & & & & \\ & & 0 & b & & & & \\ & & -b & 0 & & & & \\ & & & & 0 & b & & \\ & & & & -b & 0 & & \\ & & & & & & 0 & b' \\ & & & & & & -b' & 0 \end{pmatrix}, \tag{13}$$

$b, b' \in \mathbb{R}, \quad b \neq b', \quad b, b' \neq 0.$

It is an element of $o(6, 2)$ because it satisfies the relation $KM_1 + M_1^T K = 0$, where K is the nonsingular symmetric matrix

$$K = \begin{pmatrix} & & & -1 & & & & \\ & & 1 & & & & & \\ & 1 & & & & & & \\ -1 & & & & & & & \\ & & & & 1 & & & \\ & & & & & 1 & & \\ & & & & & & 1 & \\ & & & & & & & 1 \end{pmatrix} \tag{14}$$

with signature (6, 2). Let us denote the pairs of distinct eigenvalues of M_1 by $\alpha_1 = \pm ib$ and $\alpha_2 = \pm ib'$. They correspond to Jordan blocks of respective orders $n_1^1 = 4$, $n_2^1 = 2$, and $n_1^2 = 2$. From (8) and (9) one finds the codimensions d_1 and c_1 of the M_1 orbit and stratum

$$\begin{aligned} d_1 &= \tfrac{1}{2}[(n_1^1 + 3n_2^1 + n_1^2)] = 6, \quad t = 0, \\ c_1 &= d - \tfrac{1}{2}\nu - \delta = d - 2 = 4, \quad \delta = 0, \nu = 4. \end{aligned} \tag{15}$$

The matrix M_1 and the matrix

$$M_2 = M(b, 0) = \begin{pmatrix} 0 & b & 1 & & & & & \\ -b & 0 & & 1 & & & & \\ & & 0 & b & & & & \\ & & -b & 0 & & & & \\ & & & & 0 & b & & \\ & & & & -b & 0 & & \\ & & & & & & 0 & \\ & & & & & & & 0 \end{pmatrix}, \tag{16}$$

$0 \neq b \in \mathbb{R}$

have the same centralizers in $o(6, 2)$, as can be verified by direct computation. In this case d_1 and c_1 are given by (8) and (11), where $n_1^1 = 4$, $n_2^1 = 2$, $N_1 = N_2 = 1$, $t = 2$, $\delta = +1$, $\epsilon = +1$, $\nu = 2$. Thus one has as before $d_1 = 6$ and $c_1 = 4$. Clearly M_1 and M_2 belong to the same stratum. If, however, we put $b = b'$ in (13) the matrix $M_3 = M(b, b)$ belongs to a different $o(6, 2)$-stratum. Indeed, then we have $n_1^2 = 0$, $n_3^1 = 2$, and $\nu = 2$, so that

$$\begin{aligned} d &= \tfrac{1}{2}(n_1^1 + 3n_2^1 + 5n_3^1) = 10, \\ c &= d - \tfrac{1}{2}\nu = 9. \end{aligned} \tag{17}$$

As another example consider the matrix

$$M = \begin{pmatrix} a & 1 & & \\ & a & & \\ & & -a & \\ & & -1 & -a \end{pmatrix}, \quad a \in \mathbb{R}. \tag{18}$$

It is an element of $o(2, 2)$ because $MK + KM^T = 0$, where K is a nonsingular symmetric matrix

$$K = \begin{pmatrix} & & 1 & 0 \\ & & 0 & 1 \\ 1 & 0 & & \\ 0 & 1 & & \end{pmatrix} \tag{19}$$

of signature (2, 2). The Jordan normal form M_J of M is

$$M_J = \begin{pmatrix} a & 1 & & \\ & a & & \\ & & -a & 1 \\ & & & -a \end{pmatrix} \tag{20}$$

Using again (8) and (11) and the properties of M_J, one can determine the codimensions d and c of the orbit and stratum containing M, namely, $\alpha_1 = a$, $\alpha_2 = -a$, $\nu = 2$, $\delta = 0$, $n_1^1 = 2$, $n_1^2 = 2$, therefore

$$\begin{aligned} d &= \tfrac{1}{2}(n_1^1 + n_1^2) = 2, \\ c &= d - \tfrac{1}{2}\nu = 1. \end{aligned} \tag{21}$$

It is important to notice that a simple eigenvalue never contributes to the value of the codimension of a stratum; such an eigenvalue contributes 1 to both d and to the number of continuous parameters. As a consequence, for instance, a matrix with one 2×2 Jordan block and all other eigenvalues distinct always belongs to a stratum of codimension $c = 1$ in

$gl(n, \mathbb{C})$ regardless of the value of $n \geqslant 2$. That explains why it is simpler to work with codimensions rather than with dimensions.

As a consequence of Eqs. (3)–(11) we have the following:

Theorem: Let M be an element of a real classical Lie algebra A. The dimension (codimension) of the orbit and stratum of A containing M is determined by the Jordan normal form of M in $gl(n, \mathbb{C})$ if $A = u(p, q), o(n, \mathbb{C})$ or $sp(2n, \mathbb{C})$, in $gl(n, \mathbb{R})$ if $A = o(p, q)$ or $sp(2n, \mathbb{R})$, and in $gl(n, \mathbb{H})$ if $A = o^*(2n)$ or $sp(2p, 2q)$.

3. LOCAL STRATIFICATION OF A LIE ALGEBRA

Here we describe the stratification of a Lie algebra in the neighborhood of a singular element M_0 belonging to a stratum of codimension $c > 0$. This stratification is a direct product of a stratification in $\mathbb{C}^c$ (resp. $\mathbb{R}^c$) with $\mathbb{C}^{N-c}$ (resp. $\mathbb{R}^{N-c}$), where N is the dimension of the Lie algebra. Hence the stratification depends essentially only on c. Consequently the problem reduces to a stratification in $\mathbb{C}^c$ (resp. $\mathbb{R}^c$). To find the stratification, one computes a matrix $M(\lambda)$ depending holomorphically (smoothly) on complex (resp. real) parameters $\lambda = (\lambda_1,...,\lambda_c)$ and such that $M(0) = M_0$, the different values of λ representing all strata appearing in a neighborhood of M_0. The matrix $M(\lambda)$ is computed from a versal deformation of M_0 (cf. Refs. 7–10). One can decide from the characteristic polynomial of $M(\lambda)$ and its discriminant when singularities occur. The set of parameters $(\lambda_1,...,\lambda_c)$ corresponding to the singularities is called the *bifurcation diagram*. For $c = 1, 2$ and 3 it is convenient to draw the bifurcation diagram.

We consider two examples of bifurcation diagrams in the neighborhood of the two singularities of codimension $c = 2$ present in $u(p, q)$. The first one corresponds to the 3×3 Jordan block with the eigenvalues ib. Then

$$M(\lambda) = \begin{pmatrix} ib & 1 & 0 \\ \lambda_1 & ib & 1 \\ i\lambda_2 & \lambda_1 & ib \end{pmatrix}, \quad b, \lambda_1, \lambda_2 \in \mathbb{R}. \tag{22}$$

$M(\lambda)$ belongs to $u(2, 1)$ since

$$M(\lambda)K + KM(\lambda)^+ = 0, \quad K = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \tag{23}$$

The characteristic polynomial of $M(\lambda)$ is $(t - ib)^3 - 2\lambda_1(t - ib) - i\lambda_2$. The matrix $M(\lambda)$ is singular iff the discriminant of its characteristic polynomial is equal to zero, i.e.,

$$32\lambda_1^3 + 27\lambda_2^2 = 0. \tag{24}$$

The bifurcation diagram is shown in Fig. 1(a). The product of this diagram with R^{p+q} gives the stratification of $u(p + 2, q + 1)$ in the neighborhood of an element having one triple eigenvalue and the remaining ones simple. Hence on this diagram one readily sees the strata of $u(p + 2, q + 1)$ surrounding the singularity. Namlely, there are two open strata [on the left and on the right of the curve (24)], one closed stratum at the origin, and one stratum given by Eq. (24) minus the origin.

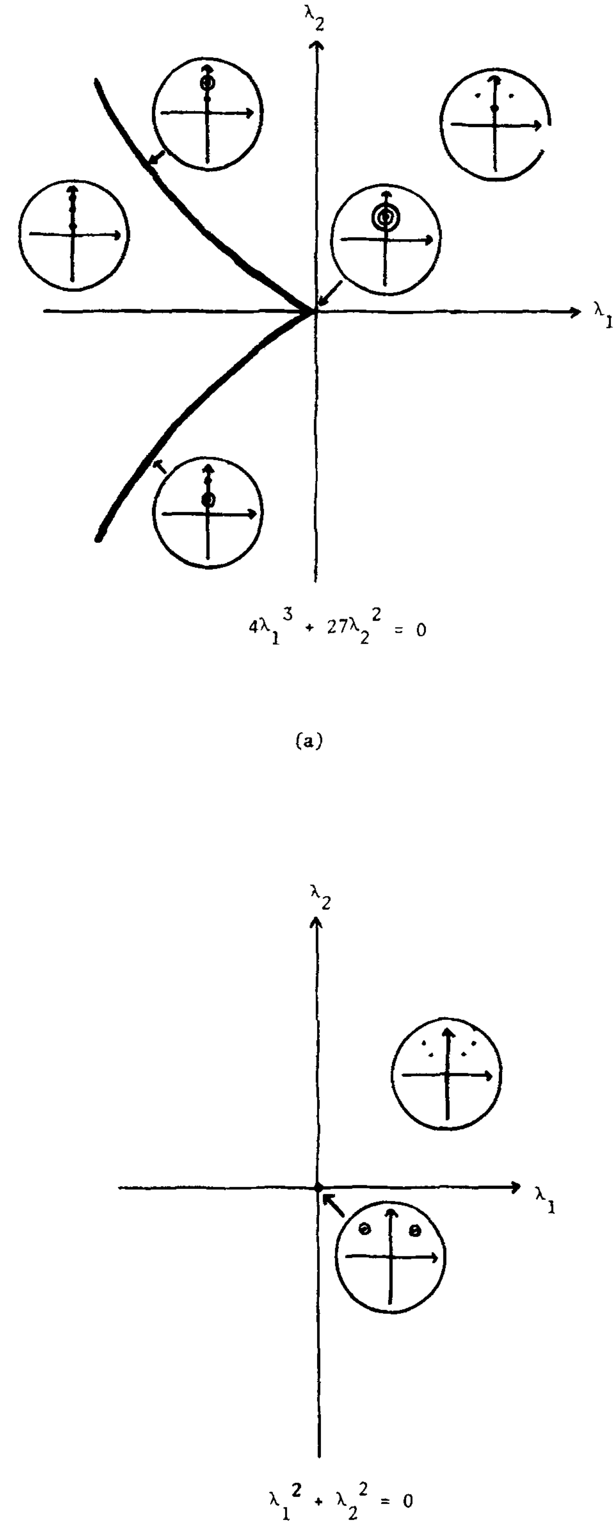

FIG. 1. Bifurcation diagrams describing the neighborhood of the singular elements of the algebra $u(p, q)$ with codimension $c = 2$. Different circles indicate the position of the eigenvalues in each region of the (λ_1, λ_2)-plane. The interior of the circles are portions of the complex plane, dots and concentric circles indicating multiple eigenvalues with the corresponding multiplicity.

The second singularity of codimension $c=2$ in $u(p, q)$ corresponds to a couple of double eigenvalues $\beta, -\beta^*$. One can take $M(\lambda)$ as

$$M(\lambda)=\begin{pmatrix} \beta & 1 & 0 & 0 \\ \lambda_1+i\lambda_2 & \beta & 0 & 0 \\ 0 & 0 & -\beta^* & -\lambda_1-i\lambda_2 \\ 0 & 0 & -1 & -\beta^* \end{pmatrix}. \quad (25)$$

It belongs to $u(2, 2)$ because it satisfies the identity

$$M(\lambda)K+KM(\lambda)^+=0, \quad K=\begin{pmatrix} 0 & I_2 \\ I_2 & 0 \end{pmatrix}. \quad (26)$$

$M(\lambda)$ is singular iff $\lambda_1^2+\lambda_2^2=0$ (cf. Fig. 1b). Similarly as in the previous case this singularity appears in any $u(p+2, q+2), p, q=0, 1,...$

Note that in $u(p, q)$ there are other singularities of codimension 2: they occur as intersections of two singularities of codimension 1, corresponding to different eigenvalues.

4. CONCLUDING REMARKS

(1) Codimensions of all orbits and strata in classical real or complex Lie algebras of all ranks are found in Eqs. (3)–(11) of Sec. 2.

(2) In applications one is often interested in particular orbits or strata, such as open or closed strata, critical orbits.

Open strata have codimension 0. There is a unique open dense stratum in complex Lie algebras and in the compact real forms. In general a noncompact real Lie algebra may have several open strata; cf. Fig. 1(a) where we have two open strata.

Closed strata are strata of maximal codimension. They are algebraic submanifolds. In the adjoint representation there is a unique closed stratum and two cases can appear:

(i) All elements of the Lie algebra have trace zero. Then the closed stratum has a unique orbit which is therefore critical (i.e., isolated in its stratum[2]). This orbit is just a point: the zero element.

(ii) In other cases [$gl(n, \mathbb{C}), gl(n, \mathbb{R}), gl(n, \mathbb{H}), u(p, q)$] the closed stratum consists of multiples of the identity matrix. Therefore there is no critical orbit.

In general, orbits are semialgebraic submanifolds.

One can remark that our definition of stratum coincides with the one of Refs. 1–3, namely: a stratum is a union of orbits having conjugate little groups.

(3) In other applications, for example the study of simple singularities, one is interested in regular and subregular elements of Lie algebras.

An element of a semisimple Lie algebra is *regular* iff its orbit has codimension R, where R is the rank of the algebra. The set of regular elements is open and dense.[5] It contains in particular all open strata and a unique orbit of nilpotent elements. An element is regular iff its characteristic polynomial coincides with its minimal polynomial.[4]

An element is *subregular* iff its orbit has codimension $N+2$, where N is the rank of the algebra. (There are no orbits of codimension $N+1$.) The set of subregular elements is a nonsingular submanifold of codimension 3 (Ref. 5). There is a unique orbit of subregular nilpotent elements.[5]

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Application of a new functional expansion to the cubic anharmonic oscillator

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A new representation of causal functionals is introduced which makes use of noncommutative generating power series and iterated integrals. This technique allows the solutions of nonlinear differential equations with forcing terms to be obtained in a simple and natural way. It generalizes some properties of Fourier and Laplace transforms to nonlinear systems and leads to effective computations of various perturbative expansions. Illustrations by means of the cubic anharmonic oscillator are given in both the deterministic and the stochastic cases.

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INTRODUCTION

Recently a new approach to causal functionals was proposed using noncommutative variables and iterated integrals.[1] This algebraic viewpoint enables us to obtain in closed form solutions of nonlinear differential equations with forcing terms. This can be done in a very simple and natural way using the vector fields connected with the equation. The rules for manipulating noncommutative variables, where the product is replaced by the shuffle, generalize Heaviside symbolic calculus to the nonlinear domain, i.e., noncommutative variables allow us to extend some properties of Laplace and Fourier transforms to nonlinear systems.

The aim of this paper is to illustrate this theory, which has appeared in engineering, by some physical examples. After some necessary recapitulation, we compare the fundamental formula giving the solution of a nonlinear differential equation with some recent attempts due to Uzes,[2] Jouvet and Phythian,[3] and Langouche *et al.*[4] Morton and Corrsin[5] used Fourier transforms for giving the solution of the cubic anharmonic oscillator, commonly known as the Duffing equation. Their computations, which had only an heuristic value, are completely justified with our noncommutative variables.

The last section is devoted to the study of statistical properties of the output of the cubic anharmonic oscillator driven by a Gaussian white noise. Noncommutative variables give a systematic understanding of the derivation of the first perturbative terms of the moments and lead to an easy implementation on computers.[6]

I. NONCOMMUTATIVE GENERATING POWER SERIES

A. Free monoid and noncommutative formal power series

Let X^* be the *free monoid*[7] generated by a finite set $X = \{x_0, \ldots, x_n\}$ called the *alphabet*. Every element of X^* is a *word* and consists of a finite sequence $x_{j_\nu} \cdots x_{j_0}$ of letters of the alphabet. The product of two words $x_{j_\nu} \cdots x_{j_0}$ and $x_{k_\mu} \cdots x_{k_0}$ is the concatenation $x_{j_\nu} \cdots x_{j_0} x_{k_\mu} \cdots x_{k_0}$. This operation is noncommutative. The neutral element is called the *empty word* and written with 1.

Let $\mathbb{R}\langle X\rangle$ and $\mathbb{R}\langle\langle X\rangle\rangle$ be the $\mathbb{R}$-algebras of formal polynomials and power series (ps) with real coefficients and noncommutative variables $x_j \in X$. An element $s \in \mathbb{R}\langle\langle X\rangle\rangle$ is written as a formal sum

$$s = \sum \{(s, w)w \mid w \in X^*\}, \quad \text{where } (s, w) \in \mathbb{R}.$$

Addition and (Cauchy) multiplication are defined by[8]

$$s_1 + s_2 = \sum \{[(s_1, w) + (s_2, w)]w \mid w \in X^*\},$$

$$s_1 s_2 = \sum \left\{\left[\sum_{w_1 w_2 = w} (s_1, w_1)(s_2, w_2)\right] w \mid w \in X^*\right\}.$$

B. Iterated integrals and analytic causal functionals

Let $\xi_0, \xi_1, \ldots, \xi_n : [0, T] \to \mathbb{R}$ be $n+1$ continuous functions with bounded variations. We define the *iterated integral*[9] $\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}$ $(0 \leqslant t \leqslant T)$ by induction on the length

$$\int_0^t d\xi_j = \xi_j(t) - \xi_j(0) \quad (j = 0, 1, \ldots, n),$$

$$\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0} = \int_0^t d\xi_{j_\nu}(\tau) \int_0^\tau d\xi_{j_{\nu-1}} \cdots d\xi_{j_0},$$

where the last integral is a Stieltjes integral.

To the inputs $u_1, \ldots, u_n : [0, T] \to \mathbb{R}$, which are assumed to be piecewise continuous, one associates the iterated integral

$$\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}, \text{ where } \xi_0(\tau) = \tau,\ \xi_i(\tau) = \int_0^\tau u_i(\sigma) d\sigma \quad (i = 1, \ldots, n).$$

Now consider a noncommutative ps $g \in \mathbb{R}\langle\langle X\rangle\rangle$. It defines a causal, or nonanticipative, functional[10] of the inputs u_i if we replace the word $x_{j_\nu} \cdots x_{j_0}$ by the corresponding iterated integral $\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}$. Thus, the numerical value[11] is

$$y(t; u_1, \ldots, u_n) = (g, 1) + \sum_{\nu \geqslant 0} \sum_{j_0, \ldots, j_\nu = 0}^{n} (g, x_{j_\nu} \cdots x_{j_0}) \times \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}. \tag{1}$$

Such a causal functional is said to be *analytic* with the *generating ps* g.

C. Fundamental formula

Consider the following differential system, which is assumed to be of first order without loss of generality,

$$\begin{cases} \dot{q}(t)(= dq/dt) = A_0(q) + \sum_{i=1}^{n} u_i(t) A_i(q), \\ y(t) = h(q). \end{cases} \tag{2}$$

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The state q belongs to a real analytic manifold Q [the initial state $q(0)$ is given]; the vector fields $A_0, A_1, \ldots, A_n$ and the function $h: Q \rightarrow \mathbb{R}$ are analytic. The inputs (or controls) $u_1, \ldots, u_n: [0, T] \rightarrow \mathbb{R}$ are often forces.

Take some local coordinates chart, where $q = (q^1, \ldots, q^N)$ and

$$A_j = \sum_{k=1}^{N} \theta_j^k (q^1, \ldots, q^N) \frac{\partial}{\partial q^k}$$

(the θ_j^k are analytic functions of $q^1, \ldots, q^N$). Recall then that the first line of (2) is equivalent to

$$\dot{q}^k(t) = \theta_0^k + \sum_{i=1}^{n} u_i(t)\theta_i^k \quad (k = 1, \ldots, N).$$

One can prove that the output y of (2) is an analytic causal functional of $u_1, \ldots, u_n$ defined by the generating ps[12]

$$\mathfrak{g} = h|_{q(0)} + \sum_{\nu \geqslant 0} \sum_{j_0, \ldots, j_\nu = 0}^{n} A_{j_0} \cdots A_{j_\nu} h|_{q(0)} x_{j_\nu} \cdots x_{j_0} \tag{3}$$

[the notation $|_{q(0)}$ means the value at $q(0)$].

The formula (3) and its proof generalize Gröbner's work[13] on Lie series and free differential equations of the form $\dot{q}(t) = A(q)$.

Uzes[2] tried also to extend Gröbner's theory to get the solution of forced nonlinear differential equations, using Gâteaux–Fréchet's functional derivatives.[14] The latest expansions are really useful if the time t is fixed once and for all. In the dynamic case, where time varies, they lead to a more complex formulation than (3). On the other hand, Jouvet and Phythian[3] and Langouche, Roekaerts, and Tirapegui[4] used a formalized operator which does not give the generating functional in a simple form. These comparisons, and others we can make with engineering attempts,[15–17] lead us to think that for causal functionals the natural expansion is done with noncommutative generating power series.

D. Volterra series

Volterra series are until now the functional expansions most commonly used.[2,4,15–17] With only one input, one obtains

$$\begin{aligned} y(t; u_1) &= w_0(t) + \int_0^t w_1(t, \tau_1) u_1(\tau_1) d\tau_1 \\ &+ \int_0^t \int_0^{\tau_2} w_2(t, \tau_2, \tau_1) u_1(\tau_2) u_1(\tau_1) d\tau_2 d\tau_1 \\ &+ \cdots + \int_0^t \int_0^{\tau_s} \cdots \int_0^{\tau_2} w_s(t, \tau_s, \ldots, \tau_1) u_1(\tau_s) \cdots u_1(\tau_1) \\ &\times d\tau_s \cdots d\tau_1 + \cdots. \end{aligned} \tag{4}$$

Kernels here are in a triangular form; hence $t \geqslant \tau_s \geqslant \cdots \geqslant \tau_1 \geqslant 0$. One can also use the symmetric form

$$\begin{aligned} y(t; u_1) &= w_0'(t) + \int_0^t w_1'(t, \tau_1) u_1(\tau_1) d\tau_1 + \cdots \\ &+ \int_0^t \cdots \int_0^t w_s'(t, \tau_s, \ldots, \tau_1) u_1(\tau_s) \cdots u_1(\tau_1) \\ &\times d\tau_s \cdots d\tau_1 + \cdots, \end{aligned}$$

where the w_s' are symmetric functions of the variables $\tau_s, \ldots, \tau_1$. In each case the kernels are uniquely defined up to a set of measure zero.

In these expansions, the linear, quadratic, cubic, etc.,... contributions are separated.

There is, in fact, a strong relationship between Volterra series and noncommutative generating ps. One can show that a Volterra series defines an analytic causal functional if, and only if, for all $s \geqslant 0$, the kernel $w_s(t, \tau_s, \ldots, \tau_1)$ is an analytic function of $t, \tau_s, \ldots, \tau_1$.

Consider the differential system

$$\begin{cases} \dot{q}(t) = A_0(q) + u_1(t) A_1(q) \\ y(t) = h(q) \end{cases}$$

of the form (2), with only a single input. From (3), we can get the output y as a Volterra series (4), where the kernels are given by[18]

$$w_0(t) = \sum_{\nu \geqslant 0} A_0^{\nu} h|_{q(0)} \frac{t^{\nu}}{\nu!} = e^{tA_0} h|_{q(0)},$$

$$\begin{aligned} w_1(t, \tau_1) &= \sum_{\nu_0, \nu_1 \geqslant 0} A_0^{\nu_0} A_1 A_0^{\nu_1} h|_{q(0)} \frac{(t - \tau_1)^{\nu_1} \tau_1^{\nu_0}}{\nu_1! \nu_0!} \\ &= e^{\tau_1 A_0} A_1 e^{(t - \tau_1) A_0} h|_{q(0)}, \end{aligned}$$

$$\begin{aligned} w_2(t, \tau_2, \tau_1) &= \sum_{\nu_0, \nu_1, \nu_2 \geqslant 0} A_0^{\nu_0} A_1 A_0^{\nu_1} A_1 A_0^{\nu_2} h|_{q(0)} \frac{(t - \tau_2)^{\nu_2} (\tau_2 - \tau_1)^{\nu_1} \tau_1^{\nu_0}}{\nu_2! \nu_1! \nu_0!} \\ &= e^{\tau_1 A_0} A_1 e^{(\tau_2 - \tau_1) A_0} A_1 e^{(t - \tau_2) A_0} h|_{q(0)}, \\ &\vdots \end{aligned}$$

$$\begin{aligned} w_s(t, \tau_s, \ldots, \tau_1) &= \sum_{\nu_0, \ldots, \nu_s \geqslant 0} A_0^{\nu_0} A_1 \cdots A_1 A_0^{\nu_s} h|_{q(0)} \frac{(t - \tau_s)^{\nu_s} \cdots \tau_1^{\nu_0}}{\nu_s! \cdots \nu_0!} \\ &= e^{\tau_1 A_0} A_1 \cdots A_1 e^{(t - \tau_s) A_0} h|_{q(0)}. \end{aligned}$$

II. A NONCOMMUTATIVE SYMBOLIC CALCULUS

A. Presentation

The generating ps representing the solution of a forced differential system can be obtained by a noncommutative symbolic calculus which generalizes Heaviside symbolic, or operational, calculus. Rather than a general formulation,[1] we apply the method to the cubic anharmonic oscillator, i.e., the Duffing equation

$$\ddot{y}(t) + \alpha \dot{y}(t) + y(t) + \beta y^3(t) = u_1(t). \tag{5}$$

To account for the cubic term, we introduce a new operation on generating ps: we define the *shuffle product* by induction on the length of words

$$\begin{aligned} &1 ш 1 = 1, \\ &\forall x \in X, \quad x ш 1 = 1 ш x = x, \\ &\forall x, x' \in X, \quad \forall w, w' \in X^*, \\ &(xw) ш (x'w') = x[w ш (x'w')] + x'[(xw) ш w']. \end{aligned} \tag{6}$$

So the shuffle product of two words is a homogeneous polynomial, the degree of which is the sum of the length of the words. For example

$$x_0 x_1 ш x_1 x_0 = 2x_0 x_1^2 x_0 + x_0 x_1 x_0 x_1 + x_1 x_0 x_1 x_0 + 2x_1 x_0^2 x_1.$$

The shuffle product of two generating ps $\mathfrak{g}_1, \mathfrak{g}_2 \in \mathbb{R}\langle\langle X \rangle\rangle$ is given by

$$\mathfrak{g}_1 \sqcup\!\sqcup \mathfrak{g}_2 = \sum \{(\mathfrak{g}_1, w_1)(\mathfrak{g}_2, w_2) w_1 \sqcup\!\sqcup w_2 | w_1, w_2 \in X^*\}.$$

Consider now the product of two iterated integrals

$$\left(\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}\right)\left(\int_0^t d\xi_{k_\mu} \cdots d\xi_{k_0}\right).$$

An integration by parts gives

$$\int_0^t d\xi_{j_\nu}(\tau)\left[\left(\int_0^\tau d\xi_{j_{\nu-1}} \cdots d\xi_{j_0}\right)\left(\int_0^\tau d\xi_{k_\mu} \cdots d\xi_{k_0}\right)\right] + \int_0^t d\xi_{k_\mu}(\tau)\left[\left(\int_0^\tau d\xi_{j_\nu} \cdots d\xi_{j_0}\right)\left(\int_0^\tau d\xi_{k_{\mu-1}} \cdots d\xi_{k_0}\right)\right].$$

This last formula is similar to the definition (6) of the shuffle product.[19] We then have the following important result.

Theorem[20]: The product of two analytic causal functionals is a functional of the same kind, the generating power series of which is the shuffle product of the two generating power series.

Consider again (5) in the following integral form:

$$y(t) + \alpha\int_0^t y(\tau)d\tau + \int_0^t d\tau\int_0^\tau y(\sigma)d\sigma + \beta\int_0^t d\tau\int_0^\tau y^3(\sigma)d\sigma = \int_0^t d\tau\int_0^\tau u_1(\sigma)d\sigma + at + b, \tag{7}$$

where $a = \dot{y}(0) + \alpha y(0)$ and $b = y(0)$.

The previous theorem and the relationship between iterated integrals and noncommutative indeterminates allow us to write (7) in the following form:

$$\mathfrak{g} + \alpha x_0 \mathfrak{g} + x_0^2 \mathfrak{g} + \beta x_0^2 \mathfrak{g} \sqcup\!\sqcup \mathfrak{g} \sqcup\!\sqcup \mathfrak{g} = x_0 x_1 + a x_1 + b. \tag{8}$$

The algebraic equation can be solved iteratively with the fixed point theorem, according to the scheme

$$\mathfrak{g}_{i+1} + \alpha x_0 \mathfrak{g}_i + x_0^2 \mathfrak{g}_i + \beta x_0^2 \mathfrak{g}_i \sqcup\!\sqcup \mathfrak{g}_i \sqcup\!\sqcup \mathfrak{g}_i = x_0 x_1 + a x_1 + b.$$

Noncommutative variables extend some properties of Laplace–Fourier transforms to the nonlinear domain. Indeed, with the linear differential equation

$$\ddot{y} + y = u_1(t)$$

we associate for $y(0) = \dot{y}(0) = 0$, by the method described above, the generating ps

$$\mathfrak{g} + x_0^2 \mathfrak{g} = x_0 x_1,$$
$$\mathfrak{g} = (1 + x_0^2)^{-1} x_0 x_1,$$

which is analogous to the classical transfer function $1/(p^2 + 1)$.

B. An example of functional expansion

Consider again Eq. (5), seeking for small β a perturbative expansion of the form

$$y(t) = y_0(t) + \beta y_1(t) + \beta^2 y_2(t) + \cdots.$$

In a quoted paper, Morton and Corrsin,[5] to this end, used the Fourier transform. This is heuristic because there is no simple relationship between the transform of a product and a product of transforms. After briefly reviewing their work, we show that our noncommutative symbolic calculus justifies it rigorously.

Making use of harmonic analysis, the authors write y and u_1 in the form

$$y(t) = \sum_\omega Y(\omega)e^{i\omega t} \quad \text{with } Y(\omega) = \frac{1}{2T}\int_{-T}^{+T} y(t)e^{-i\omega t}dt,$$
$$u_1(t) = \sum_\omega U_1(\omega)e^{i\omega t} \quad \text{with } U_1(\omega) = \frac{1}{2T}\int_{-T}^{+T} u_1(\omega)e^{-i\omega t}dt,$$

where $[-T, +T]$ can be very large. Equation (5) becomes

$$(1 - \omega^2 + i\alpha\omega)Y(\omega) + \beta\sum_{\omega'}\sum_{\omega''} Y(\omega - \omega')Y(\omega' - \omega'')Y(\omega'') = U_1(\omega)$$

or

$$(1 - \omega^2 + i\alpha\omega)Y(\omega) + \beta \sum_{\omega_1 + \omega_2 + \omega_3 = \omega} Y(\omega_1)Y(\omega_2)Y(\omega_3) = U_1(\omega).$$

Terms of the perturbative expansion

$$Y(\omega) = Y_0(\omega) + \beta Y_1(\omega) + \beta^2 Y_2(\omega) + \cdots$$

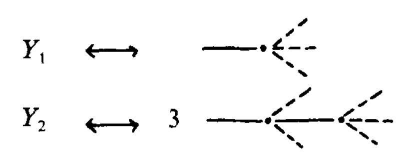
are then

$$Y_0(\omega) = (1 - \omega^2 + i\alpha\omega)^{-1} U_1(\omega) = -S(\omega)U_1(\omega),$$
$$Y_1(\omega) = S(\omega) \sum_{\omega_1 + \omega_2 + \omega_3 = \omega} Y_0(\omega_1)Y_0(\omega_2)Y_0(\omega_3),$$
$$Y_2(\omega) = 3S(\omega) \sum_{\omega_1 + \omega_2 + \omega_3 = \omega} Y_0(\omega_1)Y_0(\omega_2)Y_1(\omega_3).$$

These expressions become more and more complicated. The use of Feynman type diagrams in which

a straight line (——) represents $S(\omega)$,
a dot (.) represents β,
a dashed line (---) represents $Y_0(\omega)$,

allows us to simplify the manipulations. We deduce the following representations:



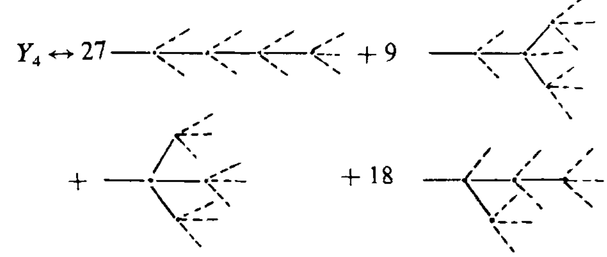
The one-to-one correspondance between Y_k and these diagrams obeys the following rules:

Four elements are joined at each vertex, at least one of which is a straight line.

There is a factor of 3 associated with every vertex having one or two dashed lines entering it.

. . . .

So to draw Y_k one must take k straight lines and k vertices, combining them in all possible ways consistent with the above rules and adding the necessary $(2k + 1) Y_0$'s (dashed lines).



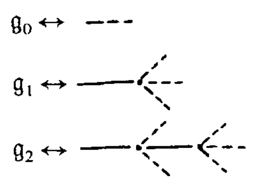
Let us write the solution $\mathfrak{g}$ of (8) in the perturbative form

$$\mathfrak{g} = \mathfrak{g}_0 + \beta\mathfrak{g}_1 + \beta^2\mathfrak{g}_2 + \cdots.$$

Hence,

$$\mathfrak{g}_0 = (1 + \alpha x_0 + x_0^2)^{-1}(x_0 x_1 + a x_0 + b)$$
$$= -S(x_0)(x_0 x_1 + a x_0 + b),$$
$$\mathfrak{g}_1 = S(x_0)\mathfrak{g}_0 ш \mathfrak{g}_0 ш \mathfrak{g}_0,$$
$$\mathfrak{g}_2 = 3S(x_0)\mathfrak{g}_0 ш \mathfrak{g}_0 ш \mathfrak{g}_1,$$

which represent them as Y_0, Y_1, Y_2 by



The connection between three branches corresponds to the shuffle of three series.[21]

III. SYSTEMS DRIVEN BY WHITE GAUSSIAN NOISES

A. Generalities

A classical problem of convergence of functional expansions arises when the inputs are white Gaussian noises. This happens with generating ps as well as with the other techniques.

As we will see in the following, it is, however, instructive to use noncommutative variables. To this end, we must first give a meaning to stochastic iterated integrals $\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}$, where the $\xi_i(t) = b_i(t)$ are Wiener processes, or Brownian motions which, for simplicity's sake, are supposed to be mutually independent and standard, i.e., $\langle b_i(t)\rangle = 0$, $\langle b_i^2(t)\rangle = |t|$. To keep the rules of ordinary calculus and taking account of approximation properties,[22] we use Stratonovich integrals.[23,24] If $\xi_0(t) = t$, $\xi_i(t) = b_i(t)$, we set

$$\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0} = \int_0^t d\xi_{j_\nu}(\tau) \int_0^\tau d\xi_{j_{\nu-1}} \cdots d\xi_{j_0},$$

where for $j_\nu \neq 0$, this last integral is a Strotonovich integral.

It is also necessary to compute the average $\langle \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0} \rangle$ of iterated integrals. The following proposition can be compared with Wick's theorem.

Proposition: The moment $\langle \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0} \rangle$ of the iterated integral $\int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}$ is given by induction on the length by

$$\left\langle \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0} \right\rangle = \begin{cases} \displaystyle\int_0^t d\tau \left\langle \int_0^\tau d\xi_{j_{\nu-1}} \cdots d\xi_{j_0} \right\rangle & \text{if } j_\nu = 0, \\ \displaystyle\int_0^t \frac{d\tau}{2} \left\langle \int_0^\tau d\xi_{j_{\nu-2}} \cdots d\xi_{j_0} \right\rangle & \text{if } j_\nu = j_{\nu-1} \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Proof: The iterated integral

$$B_{j_\nu \cdots j_0} = \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}$$

satisfies the Stratonovich stochastic differential equation

$$dB_{j_\nu \cdots j_0} = B_{j_{\nu-1} \cdots j_0} \circ d\xi_{j\nu}.$$

(For $j_\nu = 0$, i.e., $d\xi_{j\nu} = dt$, the result is trivial). This Stratonovich stochastic differential is related to that of Itô by

$$dB_{j_\nu \cdots j_0} = B_{j_{\nu-1} \cdots j_0} \cdot d\xi_{j\nu} + \tfrac{1}{2} dB_{j_{\nu-1} \cdots j_0} \cdot d\xi_{j\nu},$$

where the symbol . denotes the differential in the Itô's sense. Hence,

$$dB_{j_\nu \cdots j_0} = B_{j_{\nu-1} \cdots j_0} \cdot d\xi_{j_\nu} + \tfrac{1}{2}\big[B_{j_{\nu-2} \cdots j_0} \cdot d\xi_{j_{\nu-1}} + \tfrac{1}{2} dB_{j_{\nu-2} \cdots j_0} \cdot d\xi_{j_{\nu-1}}\big] \cdot d\xi_{j_\nu}.$$

From the definition of the Itô stochastic differentials, we have

$$\langle B_{j_{\nu-1} \cdots j_0} \cdot d\xi_{j_\nu} \rangle = 0.$$

Finally, the classical rules of stochastic calculus,

$$\begin{cases} db.db \simeq dt, \\ db.dt \simeq 0, \\ dt.dt \simeq 0, \end{cases}$$

lead to

$$\langle dB_{j_\nu \cdots j_0} \rangle = \begin{cases} \dfrac{dt}{2} \cdot \langle B_{j_{\nu-2} \cdots j_0} \rangle & \text{if } j_\nu = j_{\nu-1} \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

B. Statistics of the solutions of stochastic differential equations

Consider again the system (2); here in Stratonovich stochastic form

$$\begin{cases} dq = A_0(q)dt + \displaystyle\sum_{i=1}^n A_i(q) db_i, \\ y(t) = h(q). \end{cases}$$

$b_1, b_2, \ldots, b_n$ are standard Wiener processes, which are mutually independent [the initial state $q(0)$ is given]. Applying the previous rules to the fundamental formula, we get[25]

$$\langle y(t)\rangle = h|_{q(0)} + \sum_{\nu \geq 0} \frac{t^\nu}{\nu!}\left(A_0 + \frac{1}{2}\sum_{i=1}^n A_i^2\right)^\nu h|_{q(0)}$$
$$= \left[\exp t\left(A_0 + \frac{1}{2}\sum_{i=1}^n A_i^2\right)\right] h|_{q(0)}.$$

Example: The following system is described by

$$\begin{cases} dq = \left(B_0 + \displaystyle\sum_{i=1}^n B_i db_i\right) q(t), \\ y(t) = \lambda q(t). \end{cases}$$

The state q belongs to $\mathbb{R}^N$; B_j $(j = 0, \ldots, n)$ and λ are, respectively, square matrices and row vectors of order N (systems of this form are known, in control theory, as *regular* or *bilinear* systems). We have

$$y(t) = \lambda\left(1 + \sum_{\nu \geq 0} \sum_{j_0, \ldots, j_\nu = 0}^n B_{j_\nu} \cdots B_{j_0} \int_0^t d\xi_{j_\nu} \cdots d\xi_{j_0}\right) q(0),$$

hence

$$\langle y(t)\rangle = \lambda\left[\exp t\left(B_0 + \frac{1}{2}\sum_{i=1}^n B_i^2\right)\right] q(0). \tag{9}$$

In this particular case, we see that we have convergence and the formula (9) is then rigorous.[26]

Figure 1 gives the time expansion up to orders 8 and 12 of the moment $\langle q(t)\rangle$ where

$$\ddot{q} + \dot{q} + q + 0, 2q^3 = \dot{b}(t),$$

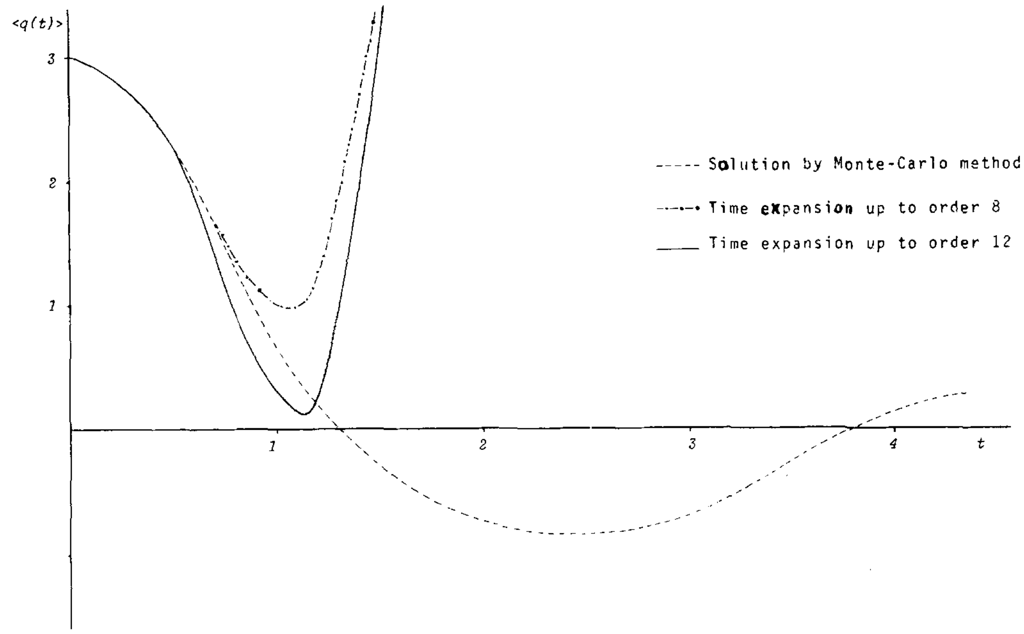


FIG. 1. First moment of the solution of the equation $\ddot{q} + \dot{q} + q + 0.2q^3 = \dot{b}(t)$ with $\sigma^2 = 5$, $q(0) = 3$, $\dot{q}(0) = 0$.

with $q(0) = 3$, $\dot{q}(0) = 0$.[27] The symbol $\dot{b}$ is the formal derivative of a Wiener process b, i.e., $\dot{b}$ is a Gaussian white noise. Here $\langle b(t)\rangle = 0$, $\langle b^2(t)\rangle = 5|t|$.

In the following we study perturbative expansions from which we can expect better results.

C. Perturbative expansions with respect to nonlinearity

Consider the nonlinear differential equation

$$Ly + \beta P(y) = \dot{b}(t) \quad (y(0), \dot{y}(0), ..., \text{are given}),$$

where L is a differential operator with constant coefficients, P a polynomial, and β a small parameter. Here we seek a perturbative expansion for the solution $y(t)$,

$$y(t) = y_0(t) + \beta y_1(t) + \beta^2 y_2(t) + \cdots. \tag{10}$$

Techniques using noncommutative variables, shown in the Appendix, give the ps g_i corresponding to the y_i:

$$g = g_0 + \beta g_1 + \beta^2 g_2 + \cdots.$$

g is the generating ps associated to y. From a result analogous to the previous proposition, it is possible to derive the first terms of the perturbative expansion of $\langle y(t)\rangle$ and more generally of $\langle y^n(t)\rangle$.

Application: We refer again to the anharmonic oscillator

$$\ddot{y} + \alpha\dot{y} + y + \beta y^3 = \dot{b}(t),$$

for which we compare our results with those of Morton and Corrsin[5] (Fig. 2). The generating ps associated with the solution y verifies the algebraic equation

$$\begin{aligned} g = & -\beta(1 + \alpha x_0 + x_0^2)^{-1} g \sqcup\!\sqcup g \sqcup\!\sqcup g \\ & + (1 + \alpha x_0 + x_0^2)^{-1}(x_0 x_1 + a x_0 + b). \end{aligned}$$

Setting

$$(1 + \alpha x_0 + x_0^2) = (1 - a_1 x_0)(1 - a_2 x_0)$$

and

$$\begin{aligned} & (1 + \alpha x_0 + x_0^2)^{-1}(ax + b) \\ & \quad = A_1(1 - a_1 x_0)^{-1} + A_2(1 - a_2 x_0)^{-1}, \end{aligned}$$

we obtain[28]

$$g_0 = \begin{array}{|ccc|} \hline 1 & 1 & \\ & 1 & 0 \\ & 0 & 0 \\ \hline \end{array}\quad \begin{array}{|ccc|} \hline 1 & 1 & \\ & 0 & 0 \\ & 1 & 0 \\ \hline \end{array}\quad \begin{array}{|cccc|} \hline 1 & X & Y & \\ & 1 & 0 & 0 \\ & 0 & 1 & 0 \\ \hline \end{array},$$

$$g_1 = \begin{array}{|cccc|} \hline 1 & X & Y & \\ & 1 & 0 & 3 \\ & 0 & 1 & 0 \\ \hline \end{array}\quad \begin{array}{|cccc|} \hline 3 & X & X & \\ & 1 & 0 & 2 \\ & 0 & 1 & 1 \\ \hline \end{array}\quad \begin{array}{|cccc|} \hline 3 & X & X & \\ & 1 & 0 & 1 \\ & 0 & 1 & 2 \\ \hline \end{array}\quad \begin{array}{|cccc|} \hline 1 & X & X & \\ & 1 & 0 & 0 \\ & 0 & 1 & 3 \\ \hline \end{array}$$

$$\begin{array}{|cccccc|} \hline 3 & X & X & X & Y & \\ & 1 & 0 & 3 & 2 & 2 \\ & 0 & 1 & 0 & 1 & 0 \\ \hline \end{array}\quad \begin{array}{|cccccc|} \hline 6 & X & X & X & Y & \\ & 1 & 0 & 2 & 1 & 1 \\ & 0 & 1 & 1 & 2 & 1 \\ \hline \end{array}$$

$$\boxed{\begin{array}{ccccc} 3 & X & X & X & Y \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 2 & 3 & 2 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 6 & X & X & X & Y & X & Y \\ 1 & 0 & 3 & 2 & 2 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 0 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 12 & X & X & X & X & Y & Y \\ 1 & 0 & 3 & 2 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 2 & 1 & 0 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 6 & X & X & X & Y & X & Y \\ 1 & 0 & 2 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 2 & 1 & 2 & 1 \end{array}}$$

$$\boxed{\begin{array}{ccccccc} 12 & X & X & X & X & Y & Y \\ 1 & 0 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 2 & 2 & 2 & 1 \end{array}}$$

For the first moment, we have then

$$\langle \mathfrak{g}_0 \rangle = \boxed{\begin{array}{ccc} 1 & 1 & \\ & 1 & 0 \\ & 0 & 0 \end{array}} \quad \boxed{\begin{array}{ccc} 1 & 1 & \\ & 0 & 0 \\ & 1 & 0 \end{array}},$$

$$\langle \mathfrak{g}_1 \rangle = \boxed{\begin{array}{ccc} 1 & X & X \\ 1 & 0 & 3 \\ 0 & 1 & 0 \end{array}} \quad \boxed{\begin{array}{ccc} 3 & X & X \\ 1 & 0 & 2 \\ 0 & 1 & 1 \end{array}} \quad \boxed{\begin{array}{ccc} 3 & X & X \\ 1 & 0 & 1 \\ 0 & 1 & 2 \end{array}} \quad \boxed{\begin{array}{ccc} 1 & X & X \\ 1 & 0 & 0 \\ 0 & 1 & 3 \end{array}}$$

$$\boxed{\begin{array}{cccccc} 12\left(\frac{\sigma^2}{2}\right) & X & X & X & X & X \\ 1 & 0 & 3 & 2 & 1 & 1 \\ 0 & 1 & 0 & 1 & 2 & 0 \end{array}} \quad \boxed{\begin{array}{cccccc} 12\frac{\sigma^2}{2} & X & X & X & X & X \\ 1 & 0 & 2 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 2 & 1 \end{array}}$$

Figure 2 gives the perturbative expansion up to order 2 of steady-state moment $\langle y^2 \rangle$.

IV. CONCLUSION

The functional methods proposed here are mathematically rigorously correct in the deterministic case, where they clarify various former attempts. In the stochastic case, their algebraic nature simplifies the computations of perturbative expansions.

APPENDIX

Consider the differential equation

$$Ly + \beta P(y) + \dot{b}(t)$$

with

$$L = \sum_{i=0}^{n} l_i \frac{d}{dt_i} \quad (l_n = 1)$$

and

$$P(x) = \sum_{j=1}^{m} p_j x^j.$$

As previously (Sec. IIA), the generating ps associated with y is given by

$$\Big(\sum_{i=0}^{n} l_i x_0^{n-i}\Big)\mathfrak{g} + x_0^n \beta \sum_{j=1}^{m} p_j \mathfrak{g}^{ш j} = x_0^{n-1}x_1 + \sum_{i=0}^{n-1} \delta_i x_0^i$$

or

$$\mathfrak{g} = -\Big(\sum_{i=0}^{n} l_i x_0^{n-i}\Big)^{-1} x_0^n \beta \sum_{j=1}^{m} p_j \mathfrak{g}^{ш j} + \Big(\sum_{i=0}^{n} l_i x_0^{n-i}\Big)^{-1}\Big(x_0^{n-1}x_1 + \sum_{i=0}^{n-1} \delta_i x_0^i\Big),$$

where $\delta_i (i = 0,...,n-1)$ are constants depending on the initial conditions.

The expansion (10) is "equivalent" to that of $\mathfrak{g}$ in powers of β:

$$\mathfrak{g} = \mathfrak{g}_0 + \beta\mathfrak{g}_1 + \beta^2\mathfrak{g}_2 + \cdots$$

with

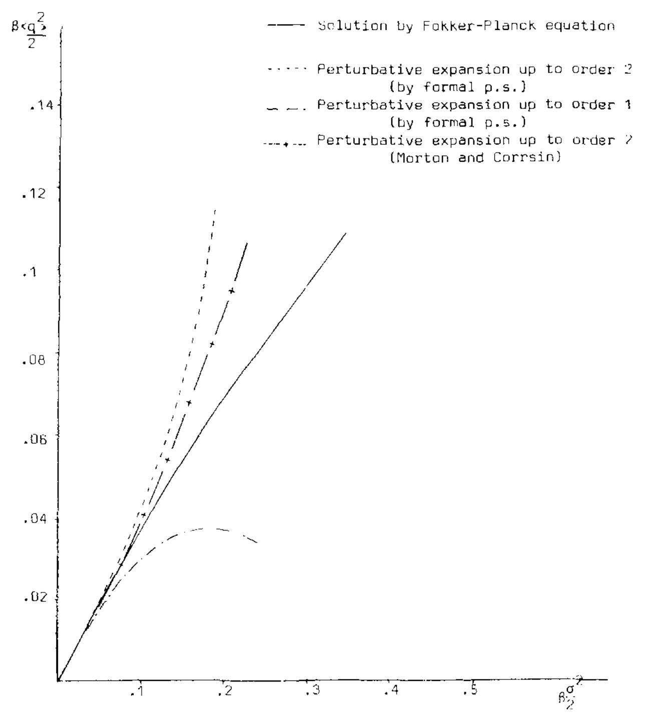


FIG. 2. Second steady-state moment of the solution of the equation $\ddot{q} + \dot{q} + q + \beta q^3 = \dot{b}(t)$, $\langle b^2(t) \rangle = \sigma^2 |t|$.

$$\mathfrak{g}_0 = \Big(\sum_{i=0}^{n} l_i x_0^{n-i}\Big)^{-1}\Big(x_0^{n-1}x_1 + \sum_{i=0}^{n-1}\delta_i x_0^i\Big)$$

and

$$\mathfrak{g}_k = -\Big(\sum_{i=0}^{n} l_i x_0^{n-i}\Big)^{-1} x_0^n \sum_{j=1}^{m} \sum_{\substack{k_1,\dots,k_j \\ k_1+\cdots+k_j=k}} p_{k_1}p_{k_2}\cdots$$

$$\times p_{k_j}\mathfrak{g}_{k_1} ш \mathfrak{g}_{k_2} ш \cdots ш \mathfrak{g}_{k_j}.$$

To have the rational expression of $\mathfrak{g}_i$, we need to compute the shuffle product of powers series of the form

$$(1-a_0x_0)^{-1}x_{i_1}(1-a_1x_0)^{-1}x_{i_2}\cdots(1-a_px_0)^{-1}. \qquad \text{(A1)}$$

Proposition[29]: Given two formal ps

$$S_1^p = (1-a_0x_0)^{-1}x_{i_1}(1-a_1x_0)^{-1}x_{i_2}\cdots x_{i_p}(1-a_px_0)^{-1} = S_1^{p-1}x_{i_p}(1-a_px_0)^{-1}$$

and

$$S_2^q = (1-b_0x_0)^{-1}x_{j_1}(1-b_1x_0)^{-1}x_{j_2}\cdots x_{j_q}(1-b_qx_0)^{-1} = S_2^{q-1}x_{j_q}(1-b_qx_0)^{-1},$$

where p and q belong to $\mathbb{N}$, the subscripts $i_1,\dots,i_p,j_1,\dots j_q$ to $\{0,1\}$, and a_i, b_j to $\mathbb{C}$; the shuffle product is given by induction on the length by

$$S_1^p ш S_2^q = (S_1^p ш S_2^{q-1})x_{j_q}[1-(a_p+b_q)x_0]^{-1} + (S_1^{p-1} ш S_2^q)x_{i_p}[1-(a_p+b_q)x_0]^{-1}$$

with

$$(1-ax_0)^{-1} ш (1-bx_0)^{-1} = [1-(a+b)x_0]^{-1}.$$

This shows that $\mathfrak{g}_i (i\geqslant 0)$ is a finite sum of expressions of the form (11). To derive perturbative expansion of the first moment,

$$\langle\mathfrak{g}\rangle = \langle\mathfrak{g}_0\rangle + \beta\langle\mathfrak{g}_1\rangle + \beta^2\langle\mathfrak{g}_2\rangle + \cdots,$$

we should compute

$$\langle(1-a_0x_0)^{-1}x_{i_1}(1-a_1x_0)^{-1}x_{i_2}\cdots x_{i_p}(1-a_px_0)^{-1}\rangle.$$

This is given (see the proposition of Sec. IIIA) by induction on the length by

$$\langle(1-a_0x_0)^{-1}x_{i_1}(1-a_1x_0)^{-1}x_{i_2}\cdots x_{i_p}(1-a_px_0)^{-1}\rangle = \begin{cases} (1-a_0x_0)^{-1}x_0\langle(1-a_1x_0)^{-1}x_{i_2}\cdots x_{i_p}(1-a_px_0)^{-1}\rangle & \text{if } i_1=0,\\ \frac{1}{2}(1-a_0x_0)^{-1}x_0\langle(1-a_2x_0)^{-1}x_{i_3}\cdots x_{i_p}(1-a_px_0)^{-1}\rangle & \text{if } i_1=i_2=1,\\ 0 & \text{otherwise.}\end{cases}$$

$\mathfrak{g}_i$ is then a rational fraction in the only variable x_0. Its decomposition into partial fractions and the following lemma give its corresponding expression in time.

Lemma: The rational fraction $(1-ax_0)^{-p}$ corresponds to the exponential polynomial

$$\Big(\sum_{j=0}^{p-1}\binom{j}{p-1}\frac{a^jt^j}{j!}\Big)e^{at}.$$

This results easily from

$$(1-ax_0)^{-p} = (1+ax_0)^{p-1} ш (1-ax_0)^{-1}.$$

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[7]Remember that the free monoid is an important subject of investigation in some questions resulting from theoretical computer science. One should cite here the name of M. P. Schützenberger. See, for example, S. Eilenberg, *Automata, Languages and Machines* (Academic, New York, 1974), Vol. A; G. Lallement, *Semigroups and Combinational Applications* (Wiley, New York, 1979).

[8]In the case $n=0$, one finds again the commutative algebras $\mathbb{R}[x_0]$ and $\mathbb{R}[[x_0]]$ of polynomials and power series in one variable.

[9]Iterated integrals have been introduced by Chen as an important tool in topology. See, for example, K. T. Chen, Bull. Am. Math. Soc. **83**, 831 (1977).

[10]A functional is said to be causal, or nonanticipative, if at time t its value depends on the values of the $u_i(\tau)$ only for $\tau < t$.

[11]Equation (1) is supposed to be absolutely convergent for t and $\max_{0,\dots,t}|u_i(\tau)|$ sufficiently small.

[12]It is worth noting that the order of subscripts in the sequences $A_{j_0}\cdots A_{j_i}h|_{q(0)}$ and $x_{j_i}\cdots x_{j_0}$ are inverted.

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[18]Here, too, the comparison with Ref. 2 is illuminating.

[19]R. Ree, Ann. Math. **68**, 210 (1958).

[20]This theorem is also essential for the proof of the fundamental formula.

[21]In addition to a justification of Morton and Corrsin's computations, we also get simple algorithms which have been implemented on computers for deriving the first terms of functional expansions (see Ref. 6). This approach can be applied to a wide range of ordinary differential equations.

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the mathematical validity of the foregoing is not ensured. This formula could also be derived, in an heuristic way, from the Fokker–Planck equation by path integral techniques. See, for example, R. L. Stratonovich, Sel. Transl. Math. Stat. Prob. **10**, 273 (1971); and R. Graham, Z. Phys. B **26**, 281 (1977).

[26]L. Arnold, *Stochastische Differentialgleichungen* (Oldenbourg, Munich, 1973); English translation, *Stochastic Differential Equations* (Wiley, New York, 1974).

[27]It should be remembered that, for this equation with an additive noise, Itô's and Stratonovich's interpretations are equivalent.

[28]The notation

$$\begin{array}{|cccccc|}\hline C & x_{i_1} & x_{i_2} & \cdots & & x_{i_p} \\ & c_{10} & c_{11} & & c_{1(p-1)} & c_{1p} \\ & c_{20} & c_{21} & & c_{2(p-1)} & c_{2p} \\ \hline \end{array}$$

means

$$CA_1^{c_{1p}}A_2^{c_{2p}}[1-(c_{10}a_1+c_{20}a_2)x_0]^{-1}x_{i_1}\cdots x_{i_p}[1-(c_{1p}a_1+c_{2p}a_2)x_0]^{-1}.$$

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Nonlinear superposition, higher-order nonlinear equations, and classical linear invariants

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We find a class of nonlinear ordinary differential equations, in ρ, of any order $m \geqslant 2$ whose solutions are given by the nonlinear superposition law $\rho(t) = x(t)r(\tau)$, $d\tau = \mu(t)dt$, where $d^m r/d\tau^m = F(r, r', \ldots)$ and $x(t)$ satisfies a special self-adjoint linear equation of order m. The coefficients of the self-adjoint equation in x, which are identical to those of the nonlinear equations in ρ, can be deduced from the well known invariants of the classical theory of linear differential equations.

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I. INTRODUCTION

The celebrated Riccati equation

$$dy/dt + a_0(t) + a_1(t)y + a_2(t)y^2 = 0 \qquad (1.1)$$

is perhaps the best known nonlinear differential equation for which a superposition principle exists. As is well known, if three distinct particular solutions y_1, y_2, and y_3 of the Riccati equation are given, its general solution follows from the algebraic relation

$$\frac{y - y_2}{y - y_1} \cdot \frac{y_3 - y_1}{y_3 - y_2} = C, \qquad (1.2)$$

where C is an arbitrary constant. This cross ratio is the composition rule for the nonlinear superposition law[1,2] for the Riccati equation. Recently, Anderson[3] has obtained a nonlinear superposition law for a system of coupled Riccati equations of the projective type, the generalized cross ratio for the ith equation being expressed in terms of particular solutions of the given system of equations. The problem of expressing the general solution of a given differential equation in terms of a fundamental set of particular solutions of that equation held the attention of certain mathematicians in the 1890's. See Anderson[3] for key references to the older literature. In the same vein, for the equation

$$dy/dt + a_0(t) + a_1(t)y + a_2(t)y^2 + a_3(t)y^3 = 0, \qquad (1.3)$$

Chiellini[4] found nonlinear superposition laws which, with certain restrictions, compose its general solution in terms of four particular solutions $y_i, i = 1,\ldots,4$.

In the foregoing cases the nonlinear superposition is such that the general solution of a given equation, or set of equations, is composed of particular solutions of the given equation, or set of equations. In contrast, we have recently studied[5,6] a different type of superposition law whereby the solution $\rho(t)$ of a certain ordinary differential equation is expressed by the composition rule

$$\rho(t) = x(t)r(\tau), \quad d\tau = dt/x^2, \qquad (1.4)$$

where x and r are solutions to differential equations related to, but different from, the given equation in ρ.

In our earlier point of view[5,6] the pair of nonlinear equations

$$\ddot\rho + p(t)\dot\rho + \omega^2(t)\rho = q_1(t)f(q_2(t)\rho), \qquad (1.5a)$$

$$\ddot x + p(t)\dot x + \omega^2(t)x = q_3(t)g(q_4(t)x), \qquad (1.5b)$$

was taken as a premise, and the nonlinear superposition law (1.4) was deduced by choosing the q's such that the ratio $r = \rho/x$ satisfied the autonomous equation $r'' = F(r)$. We will let overdots denote differentiation with respect to t and primes denote differentiation with respect to τ. The function F is determined when the q's are specified in terms of x and ρ. The choice of the q's is not unique and, in general, (1.5a) and (1.5b) become coupled. In Ref. 6 the q's were chosen to secure the pair of equations

$$\ddot\rho + p(t)\dot\rho + \omega^2(t)\rho = f(x/\rho)/(x\rho^2), \qquad (1.6a)$$

$$\ddot x + p(t)\dot x + \omega^2(t)x = g(\rho/x)/(x^2\rho), \qquad (1.6b)$$

the solution being $\rho = xr$, provided

$$r'' = F(r) = f(1/r) - g(r). \qquad (1.7)$$

We call this pair of coupled equations an Ermakov system,[6] for which there exists the first integral

$$I = \tfrac12\theta^2(\dot\rho x - \dot x\rho)^2 + \int^{x/\rho} f(\lambda)\,d\lambda + \int^{\rho/x} g(\lambda)\,d\lambda, \qquad (1.8)$$

where

$$\theta = \exp\int p(t)\,dt. \qquad (1.9)$$

The form of the right members of (1.5) may seem overly contrived at first glance, but the functional form $f(q_2\rho)$ is in fact necessary if f is to be more general than a set of powers of ρ.[5,7] We are led to this conclusion if we consider (1.5a), for example, as an equation of motion and apply Noether's theorem to the corresponding Lagrangian.[7] It was found that Noether's theorem forces the condition $q_2 = 1/x$, which is the same as our choice for the Ermakov system. From this point of view, our superposition law is a by-product of Noether's theorem.

We mention, in addition, that Noether's theorem acts to uncouple the auxiliary equation in x from the equation of motion in ρ. The Noether system

$$\ddot{\rho} + p(t)\dot{\rho} + \omega^2(t)\rho = f(x/\rho)/(x\rho^2), \tag{1.10a}$$

$$\ddot{x} + p(t)\dot{x} + \omega^2(t)x = K/(\theta^2 x^3), \tag{1.10b}$$

where K is a constant, is thus not as general as the Ermakov system. The Noether invariant for system (1.10) takes the form

$$I = \tfrac{1}{2}\theta^2(\dot{\rho}x - \dot{x}\rho)^2 + \tfrac{1}{2}K(\rho/x)^2 + \int^{x/\rho} f(\lambda)\,d\lambda. \tag{1.11}$$

Our earlier work has emphasized the importance of the invariants (1.8) and (1.11).

In this paper we forsake Ermakov systems and Noether's theorem, and thereby forfeit first integrals such as (1.8) and (1.11), in favor of a search for other nonlinear ordinary differential equations of the second and higher orders whose solutions are still given by the composition rule $\rho = xr$. We will reverse our earlier point of view and emphasis and will now regard the nonlinear superposition law

$$\rho(t) = x(t)\,r(\tau), \quad d\tau = \mu(t)\,dt, \tag{1.12}$$

as the basic premise.

In Sec. II it is seen that the linear form of the left side of (1.5a) allows the deduction of defining differential equations for both μ and x in (1.12). Linearity of the left side is assumed for all higher-order equations under consideration. In Secs. III and IV we apply (1.12) to nonlinear third- and fourth-order equations, respectively, and outline a calculational procedure to vouchsafe our superposition law. Based on these explicit calculations, inferences are drawn for the higher orders of this class of nonlinear equations and, in addition, it is noted in Sec. V that results from the classical literature are apropos to establish our composition rule for any order $m \geqslant 3$. Section VI contains several important examples of the rule. In Sec. VII we present our conclusions and indicate areas for further work.

II. SECOND-ORDER EQUATIONS

With a slight change in the notation of (1.5a) to accommodate the higher order equations, consider the second-order equation

$$\ddot{\rho} + a_1\dot{\rho} + a_2\rho = q_1 F(q_2\rho), \quad a_i = a_i(t), \quad q_i = q_i(t), \tag{2.1}$$

and the substitutions

$$\rho = x(t)\,r(\tau), \quad d\tau = \mu(t)\,dt, \tag{2.2}$$

which transform simultaneously the dependent variable ρ and independent variable t. It follows that (2.1) is transformed into

$$r'' + r'(2\mu\dot{x} + \dot{\mu}x + a_1\mu x)/(\mu^2 x)$$
$$+ r(\ddot{x} + a_1\dot{x} + a_2 x)/(\mu^2 x) = q_1 F(q_2\rho)/(\mu^2 x). \tag{2.3}$$

We make the choice to reduce this last equation to the simple autonomous form

$$r'' = F(r), \quad r' = dr/d\tau, \tag{2.4}$$

and we thus must have

$$q_1 = \mu^2 x, \quad q_2 = 1/x, \tag{2.5}$$

$$2\dot{x}/x + \dot{\mu}/\mu + a_1 = 0, \tag{2.6}$$

$$\ddot{x} + a_1\dot{x} + a_2 x = 0. \tag{2.7}$$

Let x, therefore, be a solution to (2.7), and let (2.6) serve as a defining equation for μ. Integration of (2.6) yields the solution

$$\mu\theta x^2 = 1, \quad \theta = \exp\int a_1\,dt. \tag{2.8}$$

Thus we have

$$\mu = [\theta(t)x^2(t)]^{-1}, \tag{2.9}$$

i.e., $\mu(t)$ is defined implicitly in terms of x and θ. From (2.2) the variable τ is given for the second-order case by

$$\tau = \int \frac{dt}{(\theta x^2)}. \tag{2.10}$$

Combining these results, we find for the nonlinear equation

$$\ddot{\rho} + a_1\dot{\rho} + a_2\rho = (\theta^2 x^3)^{-1} F(\rho/x), \tag{2.11}$$

the solution

$$\rho = x(t)r(\tau), \quad \tau = \int \frac{dt}{(\theta x^2)}, \tag{2.12}$$

where x is a particular solution of the linear equation (2.7) and r is the general solution of (2.4). Conversely, if x is the general solution of (2.7) then r may be a particular solution of (2.4).

Had we chosen the coefficient of r in (2.3) to be a constant K, then x would be a solution to the nonlinear equation

$$\ddot{x} + a_1\dot{x} + a_2 x = K/(\theta^2 x^3), \tag{2.13}$$

instead of (2.7), and r would satisfy

$$r'' + Kr = F(r). \tag{2.14}$$

By redefining the arbitrary function to be $F = f(1/r)/r^2$ the Noether system (1.10) is recovered. Further, by setting the coefficient of r in (2.3) equal to the arbitrary function $q_3\,g(q_4 x)$, instead of K, the Ermakov system (1.6) is regained through appropriate choices of q_3 and q_4. Thus as long as F depends only on r there is no new result for second order.

However, the substitutions (2.2) will reduce the equation

$$\ddot{\rho} + a_1\dot{\rho} + a_2\rho = (\theta^2 x^3)^{-1} F(\rho/x, \theta(\dot{\rho}x - \dot{x}\rho)), \tag{2.15}$$

to the autonomous form

$$r'' = F(r, r'), \tag{2.16}$$

by the foregoing scheme. Equation (2.15) has solution (2.12) provided x satisfies (2.7) and r now satisfies (2.16); but the system now has no Ermakov invariant, because the simple device used for integrating (2.4), i.e., multiplication by r', will not work for (2.16). It is still possible to derive[8] an equation in ρ, with autonomous equation (2.16), such that a Noether invariant will obtain.

We mention that the superposition law exhibited in this section is equivalent to the integrability condition obtained by Bandić[9] for the nonlinear equation

$$\ddot{\rho} + a_1\dot{\rho} + a_2\rho = q(x)/\rho. \tag{2.17}$$

III. THIRD-ORDER EQUATIONS

In this section we will subject the nonlinear third-order equation

$$\dddot{\rho} + 3a_2\dot{\rho} + a_3\rho = q_1 F(q_2\rho) \tag{3.1}$$

to the transformations (2.2). The result of these transformations on the left side of (3.1) is unaffected by the argument of F on the right side as long as that argument is such that F reduces to the form $F(r,r',r'',\cdots)$. For this reason, it is notationally convenient and is no loss of generality to carry only the single argument $q_2\rho$, where $q_2 = 1/x$ for all orders. It is convenient to do the calculations with the next-to-highest derivative absent from the equation. The omission of the next-to-highest derivative here and for higher orders creates no loss of generality. It is well known that the substitution $\rho = y\exp(-\int a_1\,dt)$ removes the next-to-highest derivative. It may be assumed that such substitution has been made for the equations under consideration.

When transformations (2.2) are introduced into (3.1), we easily obtain the transformed equation

$$\begin{aligned} r''' &+ 3r''(\mu^2\dot{x} + \mu\dot{\mu}x)/(\mu^3 x) \\ &+ 3r'(\mu\ddot{x} + \dot{\mu}\dot{x} + a_2\mu x + \ddot{\mu}x/3)/(\mu^3 x) \\ &+ r(\dddot{x} + 3a_2\dot{x} + a_3 x)/(\mu^3 x) = q_1 F(r)/(\mu^3 x). \end{aligned} \tag{3.2}$$

To obtain the simple autonomous equation $r''' = F(r)$, it is clear that $q_1 = \mu^3 x$ and that the coefficients of r'', r', and r must separately vanish. The latter requirement generates a set of differential equations, i.e.,

$$\dot{x}/x + \dot{\mu}/\mu = 0, \tag{3.3}$$

$$\ddot{x} + \dot{x}\dot{\mu}/\mu + x\ddot{\mu}/(3\mu) + a_2 x = 0, \tag{3.4}$$

$$\dddot{x} + 3a_2\dot{x} + a_3 x = 0. \tag{3.5}$$

These equations must be consistent or compatible. The first of these yields a defining relation for μ in terms of x, i.e.,

$$\mu = 1/x(t) \tag{3.6}$$

which expression used in (3.4) gives

$$\ddot{x} - \tfrac{1}{2}\dot{x}^2/x + \tfrac{3}{2}a_2 x = 0. \tag{3.7}$$

This last equation and (3.5) are not generally equivalent; however, they are equivalent if (3.5) is of the self-adjoint form, i.e., $2a_3 = 3\dot{a}_2$. Multiplication by x followed by integration brings the self-adjoint form of (3.5) into the second-order form (3.7). We put the integration constant equal to zero. The nonlinear equation (3.7) is equivalent to the linear equation

$$\ddot{X} + \tfrac{3}{4}a_2 X = 0, \quad X = x^{1/2}. \tag{3.8}$$

The requirement of consistency of the hierarchy (3.3)–(3.5), places a restriction on the coefficient a_3 such that the linear equation (3.5) becomes self-adjoint. With the use of (3.6), we have $q_2 = x^{-2}$. Therefore, the solution of

$$\dddot{\rho} + 3a_2\dot{\rho} + \tfrac{3}{2}\dot{a}_2\rho = x^{-2}F(\rho/x), \tag{3.9}$$

is given by $\rho = x(t)r(\tau)$, $d\tau = dt/x$, where x is a solution of the linear equation

$$\dddot{x} + 3a_2\dot{x} + \tfrac{3}{2}\dot{a}_2 x = 0, \tag{3.10}$$

and r is a solution of

$$r''' = F(r), \quad r' = dr/d\tau. \tag{3.11}$$

Alternatively, x may be determined from the second-order linear equation

$$\ddot{X} + \tfrac{3}{4}a_2 X = 0, \quad X = x^{1/2}. \tag{3.12}$$

IV. FOURTH-ORDER EQUATIONS

The next member in the class of equations under consideration is of the form

$$\rho^{(4)} + 6a_2\ddot{\rho} + 4a_3\dot{\rho} + a_4\rho = q_1 F(q_2\rho). \tag{4.1}$$

When the substitutions (2.2) are made in this equation, we will get a transformed equation of the fourth order in analogy to (3.2). To secure the autonomous equation $r^{(4)} = F(r)$, it is necessary to set separately equal to zero the coefficients of r''', r'', r', and r in the transformed equation. The following hierarchy of equations is thus produced:

$$2\frac{\dot{x}}{x} + 3\frac{\dot{\mu}}{\mu} = 0, \tag{4.2}$$

$$\ddot{x} + 2\frac{\dot{\mu}\dot{x}}{\mu} + \left(\frac{2\ddot{\mu}}{3\mu} + \frac{\dot{\mu}^2}{\mu^2} + a_2\right)x = 0, \tag{4.3}$$

$$\dddot{x} + 3\frac{\dot{\mu}\ddot{x}}{2\mu} + \left(\frac{3\ddot{\mu}}{2\mu} + 3a_2\right)\dot{x} + \left(\frac{\dddot{\mu}}{4\mu} + 3\frac{\dot{\mu}a_2}{2\mu} + a_3\right)x = 0, \tag{4.4}$$

$$x^{(4)} + 6a_2\ddot{x} + 4a_3\dot{x} + a_4 x = 0. \tag{4.5}$$

As in the previous examples, this set of differential equations must be consistent. Integration of (4.2) defines μ in terms of x, i.e.,

$$\mu = x^{-2/3}, \tag{4.6}$$

from which it follows that

$$q_1 = \mu^3 x = x^{-5/3}. \tag{4.7}$$

When this expression for μ is used in the second member, (4.3), of the heirarchy there results the equation

$$\ddot{x} - \tfrac{2}{3}\dot{x}^2/x + \tfrac{9}{5}a_2 x = 0, \tag{4.8}$$

which is equivalent to the linear equation

$$\ddot{X} + \tfrac{3}{5}a_2 X = 0, \quad X = x^{1/3}. \tag{4.9}$$

The use of (4.6) in the third member, (4.4), of the hierarchy reduces that equation to the form

$$\dddot{x} - \dot{x}\ddot{x}/x + \tfrac{4}{9}\dot{x}^3/x^2 + \tfrac{12}{5}a_2\dot{x} + \tfrac{6}{5}a_3 x = 0, \tag{4.10}$$

which is equivalent[10] to the linear equation

$$\dddot{y} + \tfrac{12}{5}a_2\dot{y} + \tfrac{4}{5}a_3 y = 0, \quad y = x^{2/3}. \tag{4.11}$$

Consistency requires this equation in y to be equivalent to the linear equation in X. The requirement is met if

$$2a_3 = 3\dot{a}_2. \tag{4.12}$$

Replacing a_3 in (4.11) by $3\dot{a}_2/2$, multiplying by y, and integrating gives

$$\ddot{y} - \tfrac{1}{2}\dot{y}^2/y + \tfrac{6}{5}a_2 y = 0, \tag{4.13}$$

which equation transforms into

$$\ddot{X} + \tfrac{3}{5}a_2 X = 0, \quad X = y^{1/2}. \tag{4.14}$$

An integration constant was set equal to zero in (4.13). The remaining equation in the hierarchy, the linear equation (4.5), must also be reducible in stages to the linear equation in X. Equation (4.5) can first be reduced to the nonlinear equation (4.10), and then by the route already indicated to linear second-order equation (4.14). To achieve the first stage, substitute (4.12) for a_3 and (4.8) for $\ddot{x}$ into (4.5); then multiply by x and integrate by parts to obtain the equation

$$x\dddot{x} - \dot{x}\ddot{x} + \tfrac{4}{9}\dot{x}^3/x + \tfrac{12}{5}a_2 x\dot{x} + \tfrac{6}{5}\dot{a}_2 x^2$$
$$+ \int \left(a_4 - \tfrac{9}{5}\ddot{a}_2 - (\tfrac{9}{5})^2 a_2^2\right) x^2 dt = 0. \tag{4.15}$$

It is readily seen that this equation is the same as (4.10) if (4.12) holds and if

$$a_4 = \tfrac{9}{5}\ddot{a}_2 + (\tfrac{9}{5})^2 a_2^2. \tag{4.16}$$

The net result of the foregoing calculations is the statement that the nonlinear fourth-order equation

$$\rho^{(4)} + 6a_2\ddot{\rho} + 6\dot{a}_2\dot{\rho} + (\tfrac{9}{5}\ddot{a}_2 + (\tfrac{9}{5})^2 a_2^2)\rho = x^{-5/3} F(\rho/x), \tag{4.17}$$

has the solution

$$\rho = x(t) r(\tau), \quad d\tau = dt/x^{2/3}, \tag{4.18}$$

where x satisfies the self-adjoint equation

$$x^{(4)} + 6a_2\ddot{x} + 6\dot{a}_2\dot{x} + (\tfrac{9}{5}\ddot{a}_2 + (\tfrac{9}{5})^2 a_2^2)x = 0, \tag{4.19}$$

and r satisfies the autonomous equation

$$d^4 r/d\tau^4 = F(r). \tag{4.20}$$

Alternatively, instead of (4.19), we may solve the second-order equation

$$\ddot{X} + \tfrac{3}{5}a_2 X = 0, \quad X = x^{1/3}. \tag{4.21}$$

V. HIGHER-ORDER EQUATIONS

The calculations made above to derive those third- and fourth-order equations with solutions given by $\rho = xr$ may easily be extended to higher-order equations of this class. We have sufficiently demonstrated the nature of the calculations to infer several conclusions valid for any order m. These are forthcoming, but first it is convenient to define the linear operator

$$L_m = \frac{d^m}{dt^m} + \binom{m}{2} a_2 \frac{d^{m-2}}{dt^{m-2}} + \binom{m}{3} a_3 \frac{d^{m-3}}{dt^{m-3}} + \cdots + a_m, \tag{5.1}$$

where $m \geqslant 2$ and $a_i = a_i(t)$, $i = 2,m$. The symbol $\binom{m}{n}$ is the usual binomial coefficient.

Given the mth-order nonlinear differential equation

$$L_m \rho = q_1 F(q_2 \rho) \tag{5.2}$$

and the transformations

$$\rho = x(t) r(\tau), \quad d\tau = \mu(t) dt, \tag{5.3}$$

there will obtain a transformed equation of the form

$$r^{(m)} + \binom{m}{1}\alpha_1 r^{(m-1)} + \binom{m}{2}\alpha_2 r^{(m-2)} + \binom{m}{3}\alpha_3 r^{(m-3)} + \cdots + \alpha_m r = q_1 F(r)/(\mu^m x). \tag{5.4}$$

The coefficients α_i are functions of x, μ, and their t derivatives and of the a_i. For each order m we choose

$$q_1 = \mu^m x, \quad q_2 = 1/x, \tag{5.5}$$

and we require the coefficients α_i separately to vanish, leaving the autonomous equation

$$d^m r/d\tau^m = F(r). \tag{5.6}$$

The set of m differential equations in x and μ thus produced must be consistent. Setting the coefficient α_1 equal to zero leads to a first-order equation in x and μ whose solution defines μ in terms of x. The vanishing of α_2 gives a nonlinear second-order equation in x and μ. We should expect that, when μ is eliminated, the resulting equation in x is then equivalent to a linear second-order equation in X via the transformation $X = x^{1/(m-1)}$. The remaining equations of the set must all reduce consistently to the linear equation in X. In the process of this reduction, restrictions are forced on the coefficients a_i, $i = 3,\ldots,m$ in such a way that the linear equation $L_m x = 0$, the last member of the set, becomes self-adjoint. Not only is the linear equation rendered self-adjoint, all coefficients higher than a_2 are determined in terms of a_2 and its derivatives. The class of nonlinear differential equations for which our superposition law will hold is thus restricted.

We therefore conclude to prove our superposition law for order m that only the first two equations of the hierarchy of equations for order m and the last, $L_m x = 0$, are needed. It is sufficient, then, to know only the first three terms of $d^m\rho/dt^m$ when it is transformed according to (5.3) to secure our nonlinear superposition law for the equation of order m of this class. It is not our intention to transform $d^m\rho/dt^m$ here; the calculation has been done by Forsyth[11] (see Sec. II of his paper). We shall be content to adapt to our notation a formulation of Rivereau,[12] whose presentation best suits our ends:

$$\rho^{(m)} = r^{(m)}\mu^m x + r^{(m-1)}\mu^{m-2}\left[\binom{m}{1}\mu\dot{x} + \binom{m}{2}\dot{\mu}x\right] + r^{(m-2)}\mu^{m-4}\left\{\binom{m}{2}\mu^2\ddot{x} + 3\binom{m}{3}\mu\dot{\mu}\dot{x} + \left[\binom{m}{3}\mu\ddot{\mu} + 3\binom{m}{4}\dot{\mu}^2\right]x\right\} + \cdots + rx^{(m)}. \tag{5.7}$$

For any order m it follows that coefficients α_1 and α_2 are given by

$$\binom{m}{1}\alpha_1 = (\mu^2 x)^{-1}\left[\binom{m}{1}\mu\dot{x} + \binom{m}{2}\dot{\mu}x\right] \tag{5.8}$$

$$\binom{m}{2}\alpha_2 = (\mu^2 x)^{-1}\left\{\binom{m}{2}\mu^2\ddot{x} + 3\binom{m}{3}\mu\dot{\mu}\dot{x} + \left[\binom{m}{3}\mu\ddot{\mu} + 3\binom{m}{4}\dot{\mu}^2\right]x + \binom{m}{2}\mu^2 x a_2\right\}. \tag{5.9}$$

Setting α_1 equal to zero yields

$$\frac{\dot{\mu}}{\mu} + \frac{2}{m-1}\frac{\dot{x}}{x} = 0, \tag{5.10}$$

and the result

$$\mu(t) = x^{2/m-1}, \tag{5.11}$$

follows for an order $m \geqslant 2$, while setting α_2 equal to zero leads to

$$\frac{\ddot{x}}{x} + (m-2)\frac{\dot{\mu}}{\mu}\frac{\dot{x}}{x} + \frac{(m-2)}{3}\frac{\ddot{\mu}}{\mu} + \frac{(m-2)(m-4)}{4}\frac{\dot{\mu}^2}{\mu^2} + a_2 = 0. \tag{5.12}$$

In view of (5.11) this last equation can be written as

$$\ddot{x}-\frac{(m-2)}{(m-1)}\frac{\dot{x}^2}{x}+3\frac{(m-1)}{(m+1)}a_2x=0, \tag{5.13}$$

which is equivalent to

$$\ddot{X}+\frac{3}{m+1}a_2X=0,\quad X=x^{1/(m-1)}, \tag{5.14}$$

for any order $m\geqslant 2$. The higher-order equations of the hierarchy corresponding to $\alpha_i=0$, $i=3,m$, must each reduce to the linear equation (5.14) for any order $m\geqslant 3$.

We are now able to state our nonlinear superposition theorem for equations of order m: For nonlinear differential equations of the form

$$\rho^{(m)}+\binom{m}{2}a_2\rho^{(m-2)}+\binom{m}{3}\tilde{a}_3\rho^{(m-3)}+\cdots+\tilde{a}_m\rho$$
$$=x^{-(m+1)/(m-1)}F(\rho/x), \tag{5.15}$$

the solution is given by

$$\rho(t)=x(t)\,r(\tau),\quad d\tau=dt/x^{2/(m-1)}, \tag{5.16}$$

where x satisfies the linear equation

$$x^{(m)}+\binom{m}{2}a_2x^{(m-2)}+\binom{m}{3}\tilde{a}_3x^{(m-3)}+\cdots+\tilde{a}_mx=0, \tag{5.17}$$

and r satisfies the autonomous equation

$$d^mr/d\tau^m=F(r). \tag{5.18}$$

The notation $\tilde{a}_i$, $i=3,\ldots,m$, indicates that the coefficients a_i are expressed in terms of a_2 and its derivatives such that (5.17) is self-adjoint. (Explicit self-adjoint forms are listed through tenth order by Chiellini.[13])

Alternatively, we can express the superposition theorem in terms of X by replacing $x^{1/(m-1)}$ with X and the mth-order linear equation (5.17) in x with the second order linear equation (5.14) in X.

Under the condition that coefficients α_1 and α_2 both vanish, Rivereau[12] has recorded the coefficients α_3, α_4, and α_5 for any order m of the transformed equation in r. Closely associated with the coefficients α_i, $i\geqslant 3$, are quantities called invariants. The first such invariant,[12] labeled B_3 here, is associated with α_3; it has the form

$$B_3=2\mu^3\alpha_3=2a_3-3\dot{a}_2. \tag{5.19}$$

The next two such invariants[12] can be written as

$$B_4=\mu^4[\alpha_4-\dot{\alpha}_3]$$
$$=a_4-2\dot{a}_3+\tfrac{6}{5}\ddot{a}_2-\frac{3(5m+7)}{5(m+1)}a_2^2, \tag{5.20}$$
$$B_5=\mu^5[\,\alpha_5-\tfrac{5}{2}\dot{\alpha}_4+\tfrac{15}{7}\ddot{\alpha}_3]$$
$$=a_5-\tfrac{5}{2}\dot{a}_4+\tfrac{15}{7}\ddot{a}_3-\frac{5(7m+13)}{7(m+1)}a_2(2a_3-3\dot{a}_2). \tag{5.21}$$

Forsyth[11] called these quantities "linear" invariants, and he carried the explicit calculations on through B_7 of this sequence. Those calcuations are rather tedious, and shall be omitted here. It is possible from the formulas given above to draw an important conclusion: The requirement that the "linear" invariants B_i, $i\geqslant 3$, vanish produces the same effect on the coefficients a_i as the requirement of consistency of resulting differential equations when the α_i are set separately equal to zero in the transformed equation in r.

As an example of the use of formulas (5.19)–(5.21), we can treat nonlinear differential equations of the form

$$\rho^{(m)}+\binom{m}{2}a_2\rho^{(m-2)}+\binom{m}{3}a_3\rho^{(m-3)}+\binom{m}{4}a_4\rho^{(m-4)}$$
$$=q_1F(q_2\rho),\quad m\geqslant 4, \tag{5.22}$$

for which the linear operator L_m truncates after the coefficient a_4. Using transformations (5.3) and deducing from $B_3=0$ and $B_4=0$ the coefficients a_3 and a_4, respectively, we find that equations of the form

$$\rho^{(m)}+\binom{m}{2}a_2\rho^{(m-2)}+\frac{3}{2}\binom{m}{3}\dot{a}_2\rho^{(m-3)}$$
$$+\binom{m}{4}\left[\tfrac{4}{5}\ddot{a}_2+\frac{3(5m+7)}{5(m+1)}a_2^2\right]\rho^{(m-4)}$$
$$=x^{-(m+1)/(m-1)}F(\rho/x),\quad m\geqslant 4 \tag{5.23}$$

have the solution $\rho=xr$, where x satisfies the linear equation which results when $F\equiv 0$ in (5.23) and r satisfies the autonomous equation $d^mr/d\tau^m=F(r)$, $m\geqslant 4$. Let us call (5.23) the four-term equation of the class. Knowledge of the set of "linear" invariants through B_n would permit determination of the coefficients a_i of the n-term equation for $m\geqslant n$. Additional examples are discussed in the next section.

VI. EXAMPLES

In this section we demonstrate the use of our superposition law with a few specific cases of the autonomous equation $r^{(m)}=F(r)$. The simplest possible form of $F(r)$, i.e., $F=0$, leads immediately to a nontrivial result. The linear equation

$$\tilde{L}_m\rho=0, \tag{6.1}$$

where $\tilde{L}_m$ is the operator L_m with the coefficients restricted to self-adjoint form in terms of a_2 and its derivatives, has the general solution

$$\rho=X_1^{m-1}(b_1+b_2\tau+\cdots+b_{m-1}\tau^{m-2}+b_m\tau^{m-1}). \tag{6.2}$$

We use the alternative form of our theorem, and X_1 is a particular solution of the linear equation (5.14). The expression in parenthesis is just the solution of $d^mr/d\tau^m=0$, and the b_i are constants of integration. Since $\tau=\int dt/X_1^2$, another solution of (5.14) is $X_2=X_1\tau$. Solution (6.2) can thus be expressed as

$$\rho=b_1X_1^{m-1}+b_2X_1^{m-2}X_2+\cdots+b_{m-1}X_1X_2^{m-2}$$
$$+b_mX_2^{m-1}. \tag{6.3}$$

Solutions of the latter type have long been known for the lower orders. Brioschi[14] seems to have been first to note this solution for third order. We will not attempt to cite all the papers since Brioschi's which report this solution for third and fourth orders. Šapkarev[15] has fairly recently found solution (6.3) for equations of orders four through eight, with and without the next-to-highest derivative. As far as we know, this solution has not been displayed before for ninth- and higher-order self-adjoint equations of the class under discussion.

Another example for any order m follows when $F(r) = K$, a constant. In this case

$$\tilde{L}_m \rho = K/X_1^{m+1}. \tag{6.4}$$

The solution is

$$\rho = K(X_2^m/X_1)/m! + \rho_c, \tag{6.5}$$

where ρ_c is solution (6.3).

An important subclass is that set of equations in ρ which are uncoupled from x or X. We posit the nonlinear equation

$$L_m \rho = K\rho^\beta, \quad K = \text{const.} \tag{6.6}$$

and ask for the value of β that will render the right member a power of r when the coefficients a_i are constrained by the requirements of our superposition rule. We find $\beta = -(m+1)/(m-1)$. Therefore the nonlinear equation

$$\tilde{L}_m \rho = K\rho^{-(m+1)/(m-1)} \tag{6.7}$$

has the general solution

$$\rho = x(t)r(\tau), \quad d\tau = dt/x^{2/(m-1)}, \tag{6.8a}$$

$$= X^{m-1}(t)r(\tau), \quad d\tau = dt/X^2, \tag{6.8b}$$

where r satisfies the autonomous equation

$$d^m r/d\tau^m = K/r^{(m+1)/(m-1)} \tag{6.9}$$

and

$$\tilde{L}_m x = 0, \quad \ddot{X} + [3/(m+1)]\, a_2 X = 0. \tag{6.10}$$

In closing our discussion of examples, we will remark on two special cases of (6.7). When $m = 2$ there results the Ermakov–Pinney[16,17] equation

$$\ddot{\rho} + a_2(t)\rho = K\rho^{-3}. \tag{6.11}$$

For this case, the autonomous equation $r'' = K/r^3$ yields the result

$$\int (b_1 - Kr^{-2})^{-1/2}\, dr = b_2 + \int \frac{dt}{x^2}, \tag{6.12}$$

the form in which Kečkić[18] implicitly left the solution $\rho = xr$. Kečkić arrived at (6.12) by a different route. But, since $\tau = \int dt/x^2$, the integration can be completed,[6] and the solution takes the form

$$\rho = [b_1 x_2^2 + 2b_2 x_1 x_2 + (b_2^2 + K)x_1^2]^{1/2}, \tag{6.13}$$

which is equivalent to the solution first found by Ermakov.[16] Functions x_1 and x_2 are linearly independent solutions of (6.10) with $m = 2$.

Gergen and Dressel[19] made a search for a third order Ermakov–Pinney equation and concluded with essentially a null result. We see for $m = 3$ in (6.7) that the third-order equation

$$\dddot{\rho} + 6a_2\dot{\rho} + 6\dot{a}_2\rho = K\rho^{-2}, \tag{6.14}$$

obtains. It is natural to call this equation *the* third-order Ermakov–Pinney equation. The solution takes the form

$$\rho = xr = (b_1 X_1^2 + b_2 X_1 X_2 + X_2^2)\, r(\tau), \tag{6.15}$$

where

$$r''' = Kr^{-2}, \quad d\tau = dt/X_1^2, \tag{6.16}$$

and X_1 and X_2 are linearly independent solutions of

$$\ddot{X} + \tfrac{3}{4} a_2 X = 0. \tag{6.17}$$

We are justified in saying that (6.7) above represents the complete Ermakov–Pinney hierarchy of equations for any order $m \geqslant 2$. It is now a simple matter to represent the general solution for $m \geqslant 2$ in the form $\rho = \rho_c r(\tau)$, where ρ_c is given by (6.3) and $r(\tau)$ is any particular solution of (6.9). In the second-order case it may be more convenient to obtain a complete solution of the r equation.

VII. CONCLUSIONS

In previous papers[5,6,8] we have considered first integrals of such systems as

$$\ddot{\rho} + a_1\dot{\rho} + a_2\rho = f(x/\rho)/(x\rho^2) \tag{7.1a}$$

and

$$\ddot{x} + a_1\dot{x} + a_2 x = g(\rho/x)/(x^2\rho) \tag{7.1b}$$

to be of an importance equal to the composition rule $\rho = xr$ for the solution. Here we have elevated the superposition law $\rho = x(t)r(\tau), d\tau = \mu(t)dt$ to the fore and have dropped consideration of first integrals altogether. In particular, the emphasis has focused on a search for those ordinary differential equations whose solutions are given by the above superposition law. We have succeeded in finding a class of equations with that property.

The class of equations found for which our superposition law is valid is of the form

$$\tilde{L}_m \rho = x^{-(m+1)/(m-1)} F(\rho/x, \dot{\rho}x - \rho\dot{x}, \cdots), \tag{7.2}$$

where $\tilde{L}_m$ is the linear operator defined in (5.1) constrained in such a way that it is self-adjoint in terms of the coefficient a_2 and its derivatives. The functions x and r satisfy the equations $\tilde{L}_m x = 0$ and $d^m r/dt^m = F(r, r', \ldots)$, respectively. We have outlined a direct calculational procedure for securing the composition rule for any order $m \neq 1$.

It is fitting at this point to note that Berkovič[20] and Berkovič and Rozov[21] have applied transformation (5.3) to nonlinear differential equations of the form

$$L_m \rho + \mu^m x F(\rho/x) = \phi(t), \tag{7.3}$$

which clearly is similar to (7.2) when $\phi(t) = 0$. Their reduction scheme, however, is considerably different from ours. For example, they require r to satisfy an mth-order *linear* autonomous equation with nonzero coefficients. Consequently, there is little overlap of their results with ours.

In pursuit of the higher-order nonlinear equations having the composition rule $\rho = xr$, we have "backed" into the rich lode of older results that exist on the invariants of linear ordinary differential equations. Many of the details of our superposition law have been known since the work of Forsyth,[11] Halphen,[22] Brioschi,[23] and others[24] and we insinuate no proprietary claims on the relation $\rho = xr$ and several other formulas of Sec. V. To our knowledge, however, the superposition law presented here has not before been applied to third- and higher-order equations. It seems to us that the classical literature pertaining to invariants of linear differential equations might now be read with an eye for application to nonlinear equations.

Generalized mth-order systems analogous to (7.1) having been neglected, the examination of third- and higher-order coupled systems for first and subsequent integrals is an open subject for further work. In addition, Noether's theorem should be applied to higher-order systems to find those with Noether symmetries.

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On one method of solving the Helmholtz equation

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This paper, Paper II of a series, presents a transformation technique that enables one to substantially simplify the form of the matrix elements of the simultaneous equations to which the two-dimensional Helmholtz equation was reduced in Paper I. The explicit passage to the limit was also carried out for the case of the normally incident wave.

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INTRODUCTION

Paper I of the present series, Ref. 1, described a new method of solution of the Helmholtz equation in domains of complex shape together with the application of this method to solution of the two-dimensional problem of plane wave diffraction on a periodical boundary of general form. The solution of this problem was obtained analytically as a series (6.12) in Paper I whose coefficients C_n, B_m had to be found from a convergent infinite system of linear algebraic equations (5.1) (Paper I). Matrix elements of this system were expressed through multiple integrals of the quasistatic Green function G, and their direct calculation on a computer would lead to a substantial increase in program complexity and computation time.

In this part of the work we shall demonstrate an analytical transformation technique that will markedly simplify the form of the matrix elements, thus decreasing multiplicity of integrals in them and even enabling to calculate several of them explicitly. Relations will be derived that permit simplifying calculations to solve the system (I.5.1), and passage to the limit when $\beta \to 0$ will be carried out for the case of normal incidence in this system. We shall make use of all notation and results of Paper I without further comment. In what follows the prefix I before a formula, e.g., (I.5.1), denotes reference to a formula in Paper I.

I. CALCULATION OF AUXILIARY INTEGRALS

Consider the function $f(z) = \exp[i\beta_n z - i\beta_p \zeta(z)]$. The function is evidently analytical in the semistrip $0 < x < d$, $y > 0$ and periodical, with the period d. Let us apply a conformal mapping $e^{2i\pi z/d} = s$. As a result the semistrip mentioned would become a unit circle c, $|s| < 1$, cut along a radius $0 < \operatorname{Re} s < 1$. Denote $f(z) = \tilde{f}(s)$. Due to periodicity in z, f as a function of s will be single-valued in the circle $|s| < 1$ and analytical throughout, except maybe the point $s = 0$, which is the image of $z = \infty$. The relations (I.3.3)–(I.3.5) imply that $\tilde{f}(s) \sim s^{n-p}$ when $s \to 0$, i.e., $\tilde{f}(0) = 0$ when $n > p$, $\tilde{f}(0) = \text{const} < \infty$ when $n = p$, and when $n < p$; then $\tilde{f}(s)$ has a pole of the order $p - n$ at zero. Thus $\tilde{f}(s)$ can be expanded into the Laurent series

$$\tilde{f}(s) = \sum_{k=n-p}^{\infty} a_k s^k.$$

From here we immediately find

$$\frac{1}{d}\int_0^d \exp[i\beta_n c - i\beta_p \zeta(x,0)]\, dx = \frac{1}{2\pi i}\int_C \tilde{f}(s)\frac{ds}{s} = a_0 = \begin{cases} 0, & n > p \\ \dfrac{1}{(p-n)!}\dfrac{d^{p-n}}{ds^{p-n}}[\tilde{f}(s)s^{p-n}]_{s=0}, & n \leqslant p. \end{cases} \tag{1.1}$$

Expressing ζ from Eq. (I.3.3) and denoting $\varphi(z) = \chi(s)$,

$$\mathscr{D}_k F(s) = \begin{cases} \dfrac{1}{k!}\dfrac{d^k}{ds^k}F(s)\Big|_{s=0}, & k \geqslant 0, \\ 0, & k < 0 \end{cases}$$

we can rewrite (1.1) in the form

$$\frac{1}{d}\int_0^d \exp[i\beta_n x - i\beta_p \zeta(x,0)]dx = \mathscr{D}_{p-n} e^{-i\beta_p \chi(s)} \equiv E_{n,p}. \tag{1.1'}$$

In the similar way we find

$$\frac{1}{d}\int_0^d \exp[i\beta_p \zeta(x,0) - i\beta_n x]dx = \mathscr{D}_{n-p} e^{i\beta_p \chi(s)} \equiv E_{\bar{n},p}. \tag{1.2}$$

Taking complex conjugates of (1.1′) and (1.2), we find two more integrals (β is assumed real):

$$\frac{1}{d}\int_0^d \exp[-i\beta_n x + i\beta_p \bar{\zeta}(x,0)]dx \quad [\mathscr{D}_{p-n} e^{-i\beta_p \chi(s)}]^* = \mathscr{D}_{p-n} e^{i\beta_p \bar{\chi}(s)} = \bar{E}_{n,p}, \tag{1.3}$$

$$\frac{1}{d}\int_0^d \exp[i\beta_n x - i\beta_p \bar{\zeta}(x,0)]dx \quad [\mathscr{D}_{n-p} e^{i\beta_p \chi(s)}]^* = \mathscr{D}_{n-p} e^{-i\beta_p \overline{\chi(s)}} = \overline{E_{\bar{n},p}}. \tag{1.4}$$

(Here and further on both an overbar and an asterisk denote complex conjugacy.)

Integrating $\tilde{f}(s)/s$ along the circumference of C_y: $|s| = e^{-2\pi y/d}$ corresponding to the segment $0 \leqslant x \leqslant d$, $\operatorname{Im} z = y$ in the z plane, we obtain an obvious generalization of (1.1′):

$$\frac{1}{d}\int_0^d \exp[i\beta_n x - i\beta_p \zeta(x,y)]dx = e^{\beta_n y} E_{n,p}. \tag{1.1''}$$

Similarly,

$$\frac{1}{d}\int_0^d \exp(-i\beta_n x + i\beta_p \zeta)dx = e^{-\beta_n y} E_{\bar{n},p}, \tag{1.2'}$$

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$$\frac{1}{d}\int_0^d \exp(-i\beta_n x + i\beta_p\bar{\xi})dx = e^{\beta_n y}\bar{E}_{n,p}, \tag{1.3'}$$

$$\frac{1}{d}\int_0^d \exp(i\beta_n x - i\beta_p\bar{\xi})dx = e^{-\beta_n y}\,\overline{E_{\bar{n},p}}. \tag{1.4'}$$

These integrals will be used while calculating the values f_n, f^+ and the matrix elements (I.5.1).

II. CALCULATION OF THE VALUES f_n, f^+

It obviously follows from (I.5.2) that to determine f_n, f^+, one needs $\hat{f}_n, \hat{f}^+$. Note that Eq. (I.5.2) was derived for $y>0$. For arbitrary $y\in\Omega$ this formula must have the form

$$f_n = e_n\theta(y) + \hat{f}_n(x,y), \tag{2.1}$$

where

$$\theta(y) = \begin{cases} 1, & y\geqslant 0, \\ 0, & y<0. \end{cases}$$

Similarly, Eq. (I.5.4) for arbitrary y has the form

$$f^+(x,y) = e_+\theta(y) + \hat{f}^+. \tag{2.1'}$$

Denote

$$\mathscr{K}_n = \int_0^d e^{i\beta_n x'} G\,|_{y'=0}dx', \quad L_n = \int_0^d e^{i\beta_n x'}\frac{\partial G}{\partial y'}\bigg|_{y'=0}dx'.$$

It follows from (I.5.2) that

$$\hat{f}_n = L_n + \alpha_n \mathscr{K}_n. \tag{2.2}$$

Similarly,

$$\hat{f}^+ = L_0 - \alpha\mathscr{K}_0. \tag{2.2'}$$

Let us apply the Green formula to a pair of functions G and $v(x',y') = e^{i\beta_n x' - |\beta_n|y'}$ in the semistrip $\Omega_H^+: 0<x'<d$, $y'>H\geqslant 0$,

$$\int_{\Omega_H^+}\int (G\Delta' v - v\Delta' G)\,dx'\,dy'$$

$$= \int_{\partial\Omega_H^+}\left(G\frac{\partial v}{\partial n'} - v\frac{\partial G}{\partial n'}\right)dl', \tag{2.3}$$

where $\Delta' = \partial^2/\partial x'^2 + \partial^2/\partial y'^2$. Taking into account the conditions (I.3.12), (I.3.14), (I.3.15) and the harmonicity of the function v, we obtain from (2.3)

$$\theta(y-h)v(x,y)$$

$$= -\int_0^d e^{i\beta_n x'}\left(\frac{\partial G}{\partial y'} + |\beta_n|G\right)_{y'=H} dx' e^{-|\beta_n|H}. \tag{2.4}$$

Hence for $H=0$ we find

$$L_n = -|\beta_n|\mathscr{K}_n - \theta(y)e^{i\beta_n x - |\beta_n|y}. \tag{2.4'}$$

Substituting Eq. (2.4) into Eqs. (2.2) and (2.2'), we obtain

$$\hat{f}_n = (\alpha_n - |\beta_n|)\mathscr{K}_n - \theta(y)e^{i\beta_n x - |\beta_n|y}, \tag{2.5}$$

$$\hat{f}^+ = -(\alpha+\beta)\mathscr{K}_0 - \theta(y)e^{i\beta x - \beta y}. \tag{2.5'}$$

Now let us apply the Green formula to the pair of functions $w_n(x',y') = e^{i\beta_n x'}\sinh\beta_n y'/\beta_n$ and G in the domain $\Omega_H: 0\leqslant x'\leqslant d, 0\leqslant y'\leqslant H$. As w_n is a harmonic function, we get

$$\iint_{\Omega_H} w_n\Delta' G\,dx'\,dy' = w_n(x,y)\chi(\Omega_H)$$

$$= \int_{\partial\Omega_H}\left(w_n\frac{\partial G}{\partial n'} - G\frac{\partial w_n}{\partial n'}\right)dl', \tag{2.6}$$

where $\chi(\Omega_H)$ is a characteristic function of the domain Ω_H. As the integrals along the segments $x=0$ and $x=d$ are cancelled because of the condition (I.3.14), and $w_n(x',0)=0$, $\partial w_n(x',0)/\partial y' = e^{i\beta_n x'}$, Eq. (2.5) implies

$$w_n(x,y)\chi(\Omega_H)$$

$$= \int_0^d e^{i\beta_n x'}\frac{\partial G}{\partial y'}\bigg|_{y'=H} dx'\,\frac{\sinh\beta_n H}{\beta_n}$$

$$- \int_0^d e^{i\beta_n x'}G\bigg|_{y'=0}dx'\cosh\beta_n H + \int_0^d e^{i\beta_n x'}G\bigg|_{y'=0}dx'.$$

Hence, using Eq. (2.4), we obtain

$$\mathscr{K}_n = w_n(x,y)\chi(\Omega_H)$$

$$+ \int_0^d e^{i\beta_n x'}G\bigg|_{y'=H}dx'\cosh\beta_n H$$

$$+ [(\sinh\beta_n H)/\beta_n]\Big[\theta(y-H)e^{i\beta_n x - |\beta_n|(y-H)}$$

$$- |\beta_n|\int_0^d e^{i\beta_n x'}G\bigg|_{y'=H}dx'\Big]. \tag{2.7}$$

Having taken H large enough with y fixed, we ensure $H>y$, $\eta'>\eta$ and obtain from Eq. (2.7)

$$\mathscr{K}_n = w_n(x,y)\theta(y) + e^{|\beta_n|H}\int_0^d e^{i\beta_n x'}G\bigg|_{y'=H}dx'$$

$$= w_n(x,y)\theta(y) - e^{|\beta_n|H}\left\{\int_0^d e^{i\beta_n x'}\left[\sum_{p=-|n|}^{|n|} e^{i\beta_p(\xi-\xi')}\right.\right.$$

$$\left.\times\frac{\cosh\beta_p\eta}{|\beta_p|d}e^{-|\beta_p|\eta'}\right]dx'$$

$$\left.+\int_0^d\left[\sum_{|p|>|n|} e^{i\beta_p(\xi-\xi')}\frac{\cosh\beta_p\eta}{|\beta_p|d}e^{-|\beta_p|\eta'}\right]_{y'=H}dx'\right\}$$

$$\equiv w_n - I_1 - I_2.$$

It follows from the estimate (I.3.5) that $I_2\to 0$ when $H\to\infty$. Thus, when $H\to\infty$, we get

$$\mathscr{K}_n = w_n(x,y)\theta(y) - e^{|\beta_n|H}\sum_{p=-|n|}^{|n|}\frac{\cosh\beta_p\eta}{|\beta_p|d}e^{i\beta_p\xi}$$

$$\times\int_0^d e^{i\beta_n x' - i\beta_p\xi' - |\beta_p|\eta'}\bigg|_{y'=H}dx' + o(1)$$

$$= w_n(x,y)\theta(y) + e^{|\beta_n|H}\left[\sum_{p=-|n|}^{-1}\frac{\cosh\beta_p\eta}{\beta_p d}\right.$$

$$\times e^{i\beta_p\xi}\int_0^d e^{i\beta_n x' - i\beta_p\xi'}\bigg|_{y'=H}dx'$$

$$\left.-\sum_{p=0}^{|n|}\frac{\cosh\beta_p\eta}{\beta_p d}e^{i\beta_p\xi}\int_0^d e^{i\beta_n x' - i\beta_p\bar{\xi}'}\bigg|_{y'=H}dx'\right] + o(1).$$

Substituting Eqs. (1.1″), (1.2′)–(1.4′) into this relation, we obtain

$$\mathscr{K}_n = w_n(x,y)\theta(y) + e^{|\beta_n|H}\left[\sum_{p=-|n|}^{-1}\frac{\cosh\beta_p\eta}{\beta_p}e^{i\beta_p\xi+\beta_n H}E_{n,p}\right.$$

$$\left.-\sum_{p=0}^{|n|}\frac{\cosh\beta_p\eta}{\beta_p}e^{i\beta_p\xi-\beta_n H}\,\overline{E_{\bar{n},p}}\right] + o(1). \tag{2.8}$$

Now consider separately the cases $n \geqslant 0$ and $n < 0$. When $n \geqslant 0$, then $p < n$ in the first sum on the right-hand side of Eq. (2.8), i.e., by definition, $E_{n,p} = 0$. Then for $n \geqslant 0$

$$\mathscr{K}_n = w_n(x,y)\theta(y) - \sum_{p=0}^{n} e^{i\beta_p\xi} \frac{\cosh\beta_p\eta}{\beta_p} \overline{E^{-}_{n,p}} + o(1).$$

As $\mathscr{K}_n$ is independent of H, we obtain finally

$$\mathscr{K}_n = w_n(x,y)\theta(y) - \sum_{p=0}^{n} e^{i\beta_p\xi} \frac{\cosh\beta_p\eta}{\beta_p} \overline{E^{-}_{n,p}}, \quad n \geqslant 0. \tag{2.9}$$

The same expression can be rewritten as

$$\mathscr{K}_n = e^{i\beta_n x} \frac{\sinh\beta_n y}{\beta_n} \theta(y) - \sum_{p=0}^{n} \frac{e^{i\beta_p\xi} + e^{i\beta_p\bar{\xi}}}{2\beta_p} \overline{E^{-}_{n,p}}, \quad n \geqslant 0. \tag{2.9'}$$

When $n < 0$, then the second sum in Eq. (2.8) equals zero, and we have

$$\mathscr{K}_n = w_n(x,y)\theta(y) + \sum_{p=n}^{-1} e^{i\beta_p\xi} \frac{\cosh\beta_p\eta}{\beta_p} E_{n,p}, \quad n < 0, \tag{2.10}$$

or

$$\mathscr{K}_n = e^{i\beta_n x} \frac{\sinh\beta_n y}{\beta_n} \theta(y) + \sum_{p=n}^{-1} \frac{e^{i\beta_p\xi} + e^{i\beta_p\bar{\xi}}}{2\beta_p} E_{n,p}, \quad n < 0. \tag{2.10'}$$

Substituting Eqs. (2.9), (2.10), or (2.9'), (2.10') into (2.5), (2.5'), we obtain explicit expressions for $\hat{f}_n$ and $\hat{f}^{+}$. The values f_n and f^{+} can be obtained now from Eq. (I.5.2').

III. SIMPLIFYING THE FORM OF g_m

In order to simplify the form of g_m, let us assume that we know such functions v_m that $\Delta v_m = -k^2 u_m$. It is not difficult to construct the systems $\{u_m\}$ for which the corresponding v_m are known. For instance, one can imbed $\mathscr{D}$ into a rectangle $0 < x < A$, $0 > y > -B$, $A \geqslant d$, $B \geqslant h$, and construct the system of $\{u_m\}$ by orthonormalizing in $\mathscr{D}$ any system of trigonometric functions that are complete in $\mathscr{D}$ [e.g., $\{\sin(k\pi x/A)\sin(l\pi y/B)\}_{k,l=1}^{\infty}$]. For such u_m the construction of v_m is obvious, One can take as u_m a complete system of eigenfunctions of the Laplace operator $\Delta u_m = -\lambda_m u_m$ in $\mathscr{D}$ (boundary conditions for all m need not coincide). Then $v_m = k^2 u_m/\lambda_m$. When the domain $\mathscr{D}$ allows the separation of variables, particular solutions (modes) of the Helmholtz equation can be taken as u_m. Then $v_m = u_m$.

Knowing v_m, one may write

$$\begin{aligned} g_m &= -k^2 \int_{\mathscr{D}}\int G u_m(x',y')\,dx'\,dy' \\ &= \int_{\mathscr{D}}\int G\Delta' v_m\,dx'\,dy' \\ &= \int_{\mathscr{D}}\int v_m \Delta' G\,dx'\,dy' + \int_{\partial\mathscr{D}} \left(G\frac{\partial v_m}{\partial n'} - v_m\frac{\partial G}{\partial n'}\right) dl' \\ &= v_m(x,y)\chi(\mathscr{D}) + \int_{\partial\mathscr{D}} \left(G\frac{\partial v_m}{\partial n'} - v_m\frac{\partial G}{\partial n'}\right) dl'. \end{aligned} \tag{3.1}$$

The expression for g_m in the form (3.1) is simpler than the original one as it contains a single instead of a double integral. It can be simplified even more if an additional condition $v_m(x,0) = 0$, $0 < x < \delta$ is imposed on v_m. Then, taking account of Eq. (I.3.13), it follows from Eq. (3.1) that

$$g_m = v_m(x,y)\chi(\mathscr{D}) + \int_{\partial\mathscr{D}} G\frac{\partial v_m}{\partial n'}\,dl'. \tag{3.1'}$$

This expression is further simplified by imposing one more condition on v_m: $\partial v_m/\partial n|_{\partial\mathscr{D}} = 0$. Then we obtain

$$g_m = v_m(x,y)\chi(\mathscr{D}) + \int_0^{\delta} G\frac{\partial v_m}{\partial y'}\bigg|_{y'=0} dx'. \tag{3.1''}$$

If we choose as v_m a system of functions satisfying the Cauchy conditions $v_m(x,0) = \partial v_m(x,0)/\partial y = 0$ on the resonator gap $0 < x < \delta$, $y = 0$, then it follows from Eq. (3.1) that

$$g_m = v_m(x,y)\chi(\mathscr{D}) + \int_{\partial\mathscr{D}} G\frac{\partial v_m}{\partial n'}\,dl'. \tag{3.1'''}$$

This form is convenient as it contains G when ζ is real, $\zeta = \xi$ since $\eta = 0$ on Γ.

If $v_m(x,0) \neq 0$, then Eq. (3.1') contains a term $\int_0^{\delta} v_m(\partial G/\partial y')|_{y'=0}dx'$ which is an integral of the double layer potential type, i.e., a discontinuous function with a gap line $0 < x < \delta$, $y = 0$. The discontinuity can be explicitly determined in the following way. Introduce a function $v'_m(x,y)$ defined in $\mathscr{D} + \partial\mathscr{D}$, harmonic in $\mathscr{D}$ and such that $v'_m(x,0) = v_m(x,0)$. Applying the Green formula to the pair G, v'_m in $\mathscr{D}$, we have

$$\begin{aligned} \int_{\mathscr{D}}\int &(G\Delta' v'_m - v'_m\Delta' G)\,dx'\,dy' \\ &= -v_m(x,y)\chi(\mathscr{D}) \\ &= \int_{\partial\mathscr{D}}\left(G\frac{\partial v'_m}{\partial n'} - v'_m\frac{\partial G}{\partial n'}\right)dl' \\ &= \int_{\partial\mathscr{D}} G\frac{\partial v'_m}{\partial n'}\,dl' - \int_0^{\delta} v'_m\frac{\partial G}{\partial y'}\bigg|_{y'=0}dx'. \\ &= \int_{\partial\mathscr{D}} G\frac{\partial v'_m}{\partial n'}\,dl' - \int_0^{\delta} v_m\frac{\partial G}{\partial y'}\bigg|_{y'=0}dx'. \end{aligned}$$

Hence

$$\int_0^{\delta} v_m\frac{\partial G}{\partial y'}\bigg|_{y'=0}dx' = v'_m(x,y)\chi(\mathscr{D}) + \int_{\partial\mathscr{D}} G\frac{\partial v'_m}{\partial n'}\,dl'. \tag{3.2}$$

The integral on the right of Eq. (3.2) has become a continuous function. The function v'_m is not uniquely determined by the conditions mentioned. Imposing additional conditions, one can obtain different versions of Eq. (3.2) in the same way as Eqs. (3.1')–(3.1''') have been obtained from Eq. (3.1).

Substituting Eq. (3.2) into Eq. (3.1), we have

$$g_m = [v_m(x,y) - v'_m(x,y)]\chi(\mathscr{D}) + \int_{\partial\mathscr{D}} G\frac{\partial(v_m - v'_m)}{\partial n'}\,dl'. \tag{3.3}$$

IV. TRANSFORMATION OF MATRIX ELEMENTS OF EQUATION (I.5.1)

Making use of the results obtained, we can substantially simplify the form of the matrix elements of the system (I.5.1).

To this end, we shall need some symmetry relations for G which immediately follow from Eq. (I.3.11):

$$G(x,y,x',y';-\beta)=G(x',y',x,y;\beta), \tag{4.1}$$

For real values of β the following relation is also valid:

$$G^*(x,y,x',y';\beta)=G(x',y',x,y;\beta). \tag{4.2}$$

The formula (I.3.11) was derived for real β, but it can be extended for complex β with a nonzero real part, if instead of $|\beta_r|$ we substitute $\tilde{\beta}_n=\beta_n\,\mathrm{sign}\,(\mathrm{Re}\beta_n)$. In the same manner Eqs. (I.5.3)–(I.5.5) are generalized to the complex β numbers. Relations (1.3), (1.4), (1.3'), (1.4') and others that follow from them are extended for complex β as a result of analytical continuation. In this case complex conjugates must be taken, regarding β as real. One has to consider complex β, for instance, in problems dealing with system eigenfields, with diffraction on a system of nonhomogeneous plane wave and with wave generation and amplification in a system with electronic flow. For calculations it is convenient to deal not with Eq. (I.5.1), but with the subsystem (I.5.1') in the form (I.5.6) together with the subsystem (I.5.1"). Consider at first coefficients of the system (I.5.1.'). Making use of Eq. (2.5), we get

$$\hat{f}_{ns}=(1/d)\int_0^d\hat{f}_n(x,0)e^{-i\beta_s x}dx$$
$$=(\alpha_n-|\beta_n|)(1/d)\int_0^d\mathscr{K}_n(x,0)e^{-i\beta_s x}dx-\delta_s^n.$$

Having used then Eqs. (2.9'), (2.10') and (1.2), (1.3), we have

$$\hat{f}_{ns}=-\delta_s^n+(\alpha_n-|\beta_n|)\begin{cases}-\displaystyle\sum_{p=0}^{n}\frac{\overline{E_{n,p}^{-}}}{2\beta_p d}\int_0^d(e^{i\beta_p\xi}+e^{i\beta_p\bar{\xi}})|_{y=0}e^{-i\beta_s x}dx, & n\geqslant 0\\ \displaystyle\sum_{p=n}^{-1}\frac{E_{n,p}}{2\beta_p d}\int_0^d(e^{i\beta_p\xi}+e^{i\beta_p\bar{\xi}})|_{y=0}e^{-i\beta_s x}dx, & n<0\end{cases}$$
$$=-\delta_s^n+(\alpha_n-|\beta_n|)\begin{cases}-\displaystyle\sum_{p=0}^{n}\frac{\overline{E_{n,p}^{-}}}{\beta_p}\frac{E_{s,p}^{-}+\overline{E_{s,p}}}{2}, & n\geqslant 0\\ \displaystyle\sum_{p=n}^{-1}\frac{E_{n,p}}{\beta_p}\frac{E_{s,p}^{-}+\overline{E_{s,p}}}{2}, & n<0\,.\end{cases} \tag{4.3}$$

Similarly it follows from Eq. (2.5') that

$$\hat{f}_s^{+}=-\delta_0^s+\frac{\alpha+\beta}{\beta}\overline{E_{0,0}^{-}}\,\frac{E_{s,0}+\overline{E_{s,0}}}{2}. \tag{4.4}$$

To simplify the form of the $\hat{g}_{ms}$ elements, change the integration order; then we have

$$\hat{g}_{ms}=\int_{\mathscr{D}}\int u_m(x',y')dx'dy'\left[(1/d)\int_0^d G(x,o,x',y')e^{-i\beta_s x}dx\right].$$

Using Eq. (4.2) (under the assumption that β is real), we get

$$\hat{g}_{ms}=\int_{\mathscr{D}}\int u_m(x',y')\,dx'dy'\left[(1/d)\int_0^d G^*(x',y',x,0)e^{-i\beta_s x}dx\right]$$
$$=\int_{\mathscr{D}}\int u_m(x',y')\,dx'dy'\left[(1/d)\int_0^d G(x',y',x,0)e^{i\beta_s x}dx\right]^*$$
$$=(1/d)\int_{\mathscr{D}}\int u_m(x,y)\mathscr{K}_s^*(x,y)\,dxdy$$
$$=\int_{\mathscr{D}}\int u_m(x,y)\left[\begin{cases}-\displaystyle\sum_{p=0}^{s}\frac{e^{-i\beta_p\xi}+e^{-i\beta_p\bar{\xi}}}{2}E_{s,p}^{-}, & s\geqslant 0\\ \displaystyle\sum_{p=s}^{-1}\frac{e^{-i\beta_p\xi}+e^{-i\beta_p\bar{\xi}}}{2}\overline{E_{s,p}}, & s<0\end{cases}\right]dx\,dy. \tag{4.5}$$

Due to analytical continuation this formula is extended for complex β [here $\overline{E}_{s,p}$ must be taken from Eq. (1.3), i.e., taking a conjugate we regard β as real]. In the same manner as Eq. (4.5) we obtain from (3.1) that

$$\hat{g}_{ms}=\int_{\partial\mathscr{D}}\left(\mathscr{K}_s^*\frac{\partial v_m}{\partial n}-v_m\frac{\partial\mathscr{K}_s^*}{\partial n}\right)dl \tag{4.6}$$

[as $y=+0$ while calculating $\hat{g}_{ms}$, one should set $\chi(\mathscr{D})=0$ in Eq. (3.1)]. It is obvious that Eqs. (3.1')–(3.1'''), (3.2), and (3.3) can be similarly rewritten.

If these relations are less convenient than Eq. (3.1), then the right-hand side of Eq. (4.6) can be somewhat simplified in the following manner. Note that $\partial\mathscr{K}_s/\partial n|_{\partial\mathscr{D}}=0$ [it follows from Eq. (I.3.2)]. Then we may write

$$\int_{\partial\mathscr{D}}v_m\frac{\partial\mathscr{K}_s^*}{\partial n}dl=\int_0^\delta v_m\left.\frac{\partial\mathscr{K}_s^*}{\partial y}\right|_{y=0}dx.$$

Then, having applied the Cauchy–Riemann relation to (2.9′), (2.10′), we get

$$\int_{\partial\mathscr{D}} v_m \frac{\mathscr{K}_s^*}{\partial n}\, dl = i\int_0^\delta v_m(x,0)\frac{\partial}{\partial x}\left[\begin{cases} -\sum\limits_{p=0}^{s} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d} E_{\bar{s},p}, & s\geqslant 0\\ \sum\limits_{p=s}^{-1} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d} \overline{E_{s,p}}, & s<0\end{cases}\right]_{y=0} dx$$

$$= iv_m(x,0)\left[\begin{cases} -\sum\limits_{p=0}^{s} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d}\Big|_{y=0} E_{\bar{s},p}, & s\geqslant 0\\ \sum\limits_{p=s}^{-1} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d}\Big|_{y=0} \overline{E_{s,p}}, & s<0\end{cases}\right]_{x=0}^{x=\delta}$$

$$-i\int_0^\delta \frac{\partial v_m(x,0)}{\partial x}\left[\begin{cases} -\sum\limits_{p=0}^{s} \dfrac{e^{i\beta_p\xi}-e^{i\beta_p\bar{\xi}}}{2\beta_p d} E_{\bar{s},p}, & s\geqslant 0\\ \sum\limits_{p=s}^{-1} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d} \overline{E_{s,p}}, & s<0\end{cases}\right]_{y=0} dx.$$

The term outside the integral on the right of this equality equals zero, as by definition $\zeta(0)=0$ and $\zeta(\delta)=\bar{\zeta}(\delta)$. Thus

$$g_{ms} = \int_{\partial\mathscr{D}} \mathscr{K}_s^* \frac{\partial v_m}{\partial n}\, dl + i\int_0^\delta \frac{\partial v_m(x,0)}{\partial x}\left[\begin{cases} -\sum\limits_{p=0}^{s} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d} E_{\bar{s},p}, & s\geqslant 0\\ \sum\limits_{p=s}^{1} \dfrac{e^{-i\beta_p\xi}-e^{-i\beta_p\bar{\xi}}}{2\beta_p d} \overline{E_{s,p}}, & s<0\end{cases}\right]_{y=0} dx. \tag{4.6′}$$

Consider now the coefficients in the system (I.5.1″). It follows from Eqs. (2.1), (2.1′), (2.5), and (2.5′) that in $\mathscr{D}$

$$f_n = (\alpha_n - |\beta_n|)\mathscr{K}_n,\quad f^+ = -(\alpha+\beta)\mathscr{K}_0.$$

By definition

$$f_{nj} = \int_{\mathscr{D}}\int u_j f_n\, dx\, dy = (\alpha_n - |\beta_n|)\int_{\mathscr{D}}\int u_j(x,y)\, dx\, dy \int_0^d G(x,y,x',0)e^{i\beta_n x'}\, dx'.$$

Let us restrict the analysis to real u_j, β and take complex conjugates to both parts of the latter equation:

$$f_{nj}^* = (\bar{\alpha}_n - |\beta_n|)\int_{\mathscr{D}}\int u_j\, dx\, dy \int_0^d G^*(x,y,x',0)e^{-i\beta_n x'}\, dx'.$$

The case of complex $u_j(x,y)$ is reduced to the one treated in the text if we consider the collection of real and imaginary parts of u_j as a new system of functions $\{\tilde{u}_m\}$.

Using Eq. (4.2) and changing places of the variables (x,y) and (x',y'), we get

$$f_{nj}^* = (\bar{\alpha}_n - |\beta_n|)\int_0^d e^{-i\beta_n x}\, dx \int_{\mathscr{D}}\int G(x,0,x',y')u_j(x',y')\, dx'\, dy' = d(\bar{\alpha}_n - |\beta_n|)\hat{g}_{jn} \quad \text{or} \quad f_{nj} = (\alpha_n - |\beta_n|)d\hat{g}_{jn}^*. \tag{4.7}$$

Similarly,

$$f_j^+ = -(\alpha+\beta)d\hat{g}_{j0}^*. \tag{4.8}$$

These formulas can be generalized to complex β in the same manner as all the above formulas, i.e., $|\beta_n|$ is substituted by $\beta_n\,\mathrm{sgn}(\mathrm{Re}\beta_n)$ and conjugates are taken to "real β."

In the similar way symmetry relations are obtained for g_{mj}:

$$g_{mj}^* = g_{jm}. \tag{4.8′}$$

Making use of the results of Sec. III and applying the Green formula, integrals in g_{mj} can be lowered by two orders, g_{mj} being expressed by a double integral of G. We present the corresponding results without intermediate steps and only for cases corresponding to Eqs. (3.1″) and (3.3)

$$g_{mj} = v_{mj} - \frac{1}{k^2}\int_0^\delta \frac{\partial v_m(x',0)}{\partial y'}\, dx' \int_0^\delta G(x,0,x',0)\frac{\partial v_j(x,0)}{\partial y}\, dx, \tag{4.9}$$

$$g_{mj} = v_{mj} - v'_{mj} - \frac{1}{k^2}\int_{\partial\mathscr{D}} \frac{\partial(v_m - v'_m)}{\partial n'}\, dl' \int_{\partial\mathscr{D}} G\frac{\partial(v_j - v'_j)}{\partial n}\, dl. \tag{4.10}$$

Here

$$v_{mj} = \int_{\mathscr{D}}\int v_m u_j\, dx\, dy,\quad v'_{mj} = \int_{\mathscr{D}}\int v'_m u_j\, dx\, dy.$$

Derivation of Eq. (4.9) and similar transformation in the rest of cases considered in Sec. III present no difficulties.

V. NORMAL INCIDENCE CASE

As it was mentioned in Ref. 1 a passage to the limit when $\beta \to 0$ must be carried out to fit the results obtained for the case of normal incidence. Directly this passage can be made only in the values $E_{n,p}, E^-_{n,p}$ (and in their conjugates). We get

$$\lim_{\beta \to 0} E_{n,p} \equiv E_{n,p}(0) = \mathscr{D}_{p-n} \exp[-2i\pi p\chi(s)/d],$$

$$E^-_{n,p}(0) = \mathscr{D}_{n-p} \exp[2i\pi p\chi(s)/d]. \tag{5.1}$$

Hence

$$E_{n,0}(0) = E^-_{n,0}(0) = \delta^0_n, \tag{5.2}$$

and, if the function $\chi(s)$ is real on the real axis, then for all p,q

$$\bar{E}_{p-q,p}(0) = E^-_{p,q}(0). \tag{5.3}$$

If only $\chi(0), \chi'(0),...,\chi^{(r)}(0)$ are real, then Eq. (5.3) is valid for all p, provided $q \leqslant r$. It follows from the symmetry principle that $\chi(s)$ is real if and only if the periodic system Ω is symmetric with respect to the axis $x = d/2$. We omit the easy proof of this fact.

Let us find now $\lim_{\beta \to 0} \beta f_n(x, y; \beta)$ and $\lim_{\beta \to 0} \beta g_m(x, y; \beta)$. After obvious transformations Eq. (5.2) yields

$$\lim_{\beta \to 0} \beta f_n = ik\delta^0_n, \quad \lim_{\beta \to 0} \beta f^+ = -ik,$$

$$\lim_{\beta \to 0} \beta g_m = -(1/d) \int_{\mathscr{S}}\int u_m \, dx \, dy. \tag{5.4}$$

Now we may find $\lim_{\beta \to 0} u_m$. To this end, we first find $\lim_{\beta \to 0} \beta u(x, y; \beta)$. Taking into account that $u(x, y; 0)$ is a finite value and using Eq. (5.4), we obtain from Eq. (I.6.12)

$$0 = -ikA + ikC_0(0) + \frac{i}{kd} \sum_{m=0}^{\infty} B_m(0) \int_{\mathscr{S}}\int u_m \, dx \, dy, \tag{5.5}$$

where $C_0|_{\beta=0} = C_0(0)$, $B_m|_{\beta=0} = B_m(0)$.

If the orthonormal system $\{u_m\}$ is chosen so that $u_0(x, y) = 1/\sqrt{S}$, where S is the area of $\mathscr{D}$, then Eq. (5.5) will acquire an especially simple form

$$C_0(0) + (i/2\kappa\pi)B_0(0) = A, \tag{5.5'}$$

where $\kappa = kd/2\pi$. Using Eq. (I.2.4), Eq. (5.5') can be written in the alternative form

$$C_0(0) + (i/2\kappa\pi) \int_{\mathscr{S}}\int u(x, y) \, dx \, dy = A, \tag{5.5''}$$

or

$$(1/d) \int_0^d u_s(x,0) \, dx + (i/2\kappa\pi) \int_{\mathscr{S}}\int u(x, y) \, dx \, dy = A. \tag{5.5'''}$$

These relations are interesting as they are, e.g., for control in numeric calculations. To take the limit at $\beta \to 0$ directly in the system (I.5.1), and therefore in the coefficients $\tilde{C}_n, \tilde{B}_n$ we need, asymptotics of the matrix elements (I.5.1) must be found at $\beta \to 0$ with the accuracy $O(\beta)$. After some transformations we find:

$$\hat{f}_{ns} = -\delta^s_n + \left(1 + \frac{ik}{\beta}\right)\delta^0_n\delta^0_s - \frac{k}{2}\delta^0_n\left[\overline{\frac{\chi^{(s)}(0)}{s!}} - \delta^0_s \overline{\chi(0)}\right] + [a_n(0) - |n|]$$
$$\times \begin{cases} -\sum_{p=1}^{n} \dfrac{\overline{E^-_{n,p}(0)}}{p} \dfrac{E^-_{s,p}(0) + E_{s,p}(0)}{2}, & n \geqslant 0 \\ \sum_{p=n}^{-1} \dfrac{E_{n,p}(0)}{p} \dfrac{E^-_{s,p} + E_{s,p}(0)}{2}, & n < 0 \end{cases} + O(\beta) \equiv \frac{ik}{\beta}\delta^0_n\delta^0_s + \hat{f}'_{ns} + O(\beta), \tag{5.6}$$

where $a_n(\beta) \equiv \alpha_n d = (b^2_n - \kappa^2)^{1/2}$, $b_n = \beta_n d/2\pi$, so that $a_n(0) = (n^2 - \kappa^2)^{1/2}$;

$$\hat{g}_{ms} = -\delta^0_s \frac{\sigma_m}{\beta d} + \int_{\mathscr{D}}\int u_m \left[\frac{i\xi}{d}\delta^0_s + \begin{cases} -\dfrac{i}{2d}\dfrac{\chi^{(s)}(0)}{s!} - \sum_{p=1}^{s} \dfrac{e^{-2i\pi\zeta/d} + e^{-2i\pi\bar{\zeta}/d}}{4\pi d} E^-_{s,p}(0), & s \geqslant 0 \\ \sum_{p=s}^{-1} \dfrac{e^{-2i\pi\zeta/d} + e^{-2i\pi\bar{\zeta}/d}}{4\pi d} \overline{E_{s,p}(0)}, & s < 0 \end{cases}\right] dx \, dy + O(\beta)$$
$$\equiv -\delta^0_s \frac{\sigma_m}{\beta d} + \hat{g}'_{ms} + O(\beta), \tag{5.7}$$

where $\sigma_m = \int\int_{\mathscr{D}} u_m \, dx \, dy$;

$$f_{sj} = d(\alpha_s - |\beta_s|)\hat{g}^*_{js} = \delta^0_s\left(1 + \frac{ik}{\beta}\right)\sigma_j + d(\alpha_s - |\beta_s|)\overline{\hat{g}'_{js}} + O(\beta), \tag{5.8}$$

$$g_{mj} = -\int_{\mathscr{D}}\int u_j \, dx \, dy \int_{\mathscr{S}}\int \left[\frac{1}{\beta d} + \frac{2(\xi - \xi') - |\eta - \eta'| - |\eta + \eta'|}{2d}\right.$$
$$\left. + \sum_{\substack{p=-\infty \\ p \neq 0}}^{\infty} e^{2i\pi(\xi - \xi')/d} \frac{e^{-2\pi|p||\eta - \eta'|/d} + e^{-2\pi|p||\eta + \eta'|/d}}{4\pi|p|}\right] u_m(x', y') \, dx' \, dy' + O(\beta) \equiv -\frac{\sigma_j\sigma_m}{\beta d} - g'_{mj} + O(\beta). \tag{5.9}$$

Further on, for the sake of simplicity, we shall consider the case when $u_0 = \text{const}$, and, therefore, $\sigma_n = \delta^0_m$ due to orthonormality of the system $\{u_m\}$. Introduce the matrix $A = ((a_{p,q}))$, $-N \leqslant p,q \leqslant N+M$, where: $a_{p,q} = \hat{f}_{p,q}$ when $|p|,|q| \leqslant N$; $a_{p,N+j+1} = f_{p,j}$ when $|p| \leqslant N$, $0 \leqslant j \leqslant M$; $a_{N+m+1,q} = \hat{g}_{mq}$ when $0 \leqslant m \leqslant M$, $|q| \leqslant N$; $a_{N+m+1,N+j+1} = g_{m,j}$ when $0 \leqslant j$, $m \leqslant M$. Having expressed the solution of the system (I.5.1) by Kramer formulas and using the relation

$$f_p^+ = \frac{2\alpha}{\beta-\alpha}\delta_0^p + \frac{\beta+\alpha}{\beta-\alpha}\hat{f}_{0,p}$$

that follows from Eqs. (2.5), (2.5′), we find after obvious transformations

$$\tilde{C}_l = \frac{2\alpha A}{\alpha-\beta}\frac{\Delta_l}{\mathscr{D}}, \quad l \neq 0, \tag{5.10}$$

$$\tilde{C}_0 = A\left(\frac{2\alpha}{\alpha-\beta}\frac{\Delta_0}{\mathscr{D}} + \frac{\alpha+\beta}{\alpha-\beta}\right), \tag{5.11}$$

$$\tilde{B}_m = \frac{2\alpha A}{\alpha-\beta}\frac{\Delta_{N+m+1}}{\mathscr{D}}, \tag{5.12}$$

where $\mathscr{D} = |d_{pq}| = \det A^T$, A^T is the transposition of the matrix A, Δ_l is a cofactor of the element d_{0l} in $\mathscr{D}$. Equations (5.10)–(5.12) permit in the general case to decrease the amount of computations when solving the system (I.5.1). Using Eqs. (5.6)–(5.9), take the limit with $\beta \to 0$ in Eqs. (5.10)–(5.12). After easy but cumbersome transformations, which have been omitted, we obtain

$$\lim_{\beta\to 0} \tilde{C}_l \equiv \tilde{C}_l(0) = 2A\Delta_{l,0}/\mathscr{D}_0, \quad (l \neq 0,\ |l| \leqslant N), \tag{5.13}$$

$$\lim_{\beta\to 0} \tilde{B}_m \equiv \tilde{B}_m(0) = 2A\Delta_{N+m+1,0}/\mathscr{D}_0, \tag{5.14}$$

where $\mathscr{D}_0 = |d'_{pq}| = detA_0^T$,

$$A_0 = ((a'_{p,q} + \delta_p^{N+1}a_{0q}/ikd - \delta_q^{N+1}a_{p0} - \delta_p^{N+1}\delta_q^{N+1}a_{pq}/ikd))_{p\neq 0,\, q\neq 0},$$

$\Delta_{l,0}$ is a cofactor of the element $d_{N+1,l}$ in $\mathscr{D}_0$,

$$a'_{p,q} = a_{p,q} - \delta_p^0\delta_q^0 d/\beta, \quad |p|,\ |q| \leqslant N,$$

$$a'_{p,N+j+1} = a_{p,N+j+1} + (ik/\beta)\delta_p^0\delta_j^0, \quad |p| \leqslant N,\ 0 \leqslant j \leqslant M,$$

$$a'_{N+m+1,q} = a_{N+m+1,q} - (1/\beta d)\delta_m^0\delta_q^0, \quad |q| \leqslant N,\ 0 \leqslant m \leqslant M,$$

$$a'_{N+m+1,N+j+1} = a_{N+m+1,N+j+1} - (1/\beta d)\delta_m^0\delta_j^0, \quad 0 \leqslant j,\ m \leqslant M.$$

Knowing $\tilde{B}_0(0)$, the coefficient $\tilde{C}_0(0)$ is determined from Eq. (5.5′), which, as can be easily seen, is valid if C_0 and B_0 in it are substituted by $\tilde{C}_0$, $\tilde{B}_0$. The exact coefficients C_m, B_m when $\beta \to 0$ are obtained, in the same way as in the general case, from $\tilde{C}_n(o)$, $\tilde{B}_m(o)$ when $N,M \to \infty$. A rigorous proof of this obvious physical fact would be a rather cumbersome one, and it will be skipped.

CONCLUSION

The relations obtained in this paper allow one to substantially simplify the form of the matrix elements in the system (I.6.2) and thus decrease the amount of computer time needed for its numerical solution. Applications of the described method for calculating diffraction on specific structures will be presented in subsequent papers.

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Pseudopotentials and Lie symmetries for the generalized nonlinear Schrödinger equation [a)]

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The generalized nonlinear Schrödinger equation $z_{xx} + iz_t = f(z, z^*)$ is analyzed from the point of view of the existence of pseudopotentials, Bäcklund transformations, Lie symmetries, and conservation laws. Applying the Wahlquist–Estabrook method of closed differential ideals we show that eight classes of nontrivial interaction terms $f(z,z^*)$ exist for which the equation allows the existence of pseudopotentials. Five of them simply lead to conservation laws, the remaining three to Bäcklund transformations. The usual "cubic" nonlinear Schrödinger equation with $f(z,z^*) = \epsilon z|z|^2$ is obtained as a special case. It is also the only case for which the Bäcklund transformation contains a free parameter. We show that the real and complex parts of this parameter are generated by the dilation and Galilei invariance of the equation.

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I. INTRODUCTION

The method of "pseudopotentials," as developed by Wahlquist and Estabrook[1–4] and others,[5–13] provides a certain unity to a variety of different solution techniques for certain classes of nonlinear differential equations. This approach includes, as special cases, the derivation of conservation laws, Bäcklund transformations, and the linear equations of the inverse scattering method. The Wahlquist–Estabrook (WE) approach, based upon the study of closed differential ideals, does not provide the most general integrable transformation equations, but it has the virtue of computational simplicity and a natural geometrical interpretation in terms of covariant derivatives with respect to integrable connections. Among the equations to which it has been applied are the KdV, modified KdV, sine (sinh)–Gordon, Liouville, and nonlinear Schrödinger equations, as well as certain other equations in more than one spatial dimension.

Another useful approach in the study of partial differential equations involves the determination of symmetries in the sense of Lie. This leads, in the case of linear equations, to solutions in separated variables and, in the nonlinear case, to classes of self-similar or invariant solutions under the action of the various symmetry groups. The method has been applied, in particular, to the classification of symmetry-breaking nonlinear interactions in the Schrödinger equation[14] as well as to the determination of invariant solutions to the Yang-Mills equations.[15–18]

A link between the study of Lie symmetries and the study of Bäcklund transformations exists in the classical case[19–21] of the sine–Gordon equation, describing pseudospherical surfaces, where it has been shown how the composition of the two gives rise to a parametric family of Bäcklund transformations. This interpretation of the parameters occurring in Bäcklund transformations was generalized by Sasaki[22] to other equations admitting symmetries of the dilation type. The existence of such parametric families is of central importance in the applicability of Bäcklund transformations to the generation of new solutions from old, since they underlie the existence of a permutability theorem or double Bäcklund transformation.[1,2]

In this work, we generalize some of the results of Estabrook and Wahlquist concerning the nonlinear Schrödinger equation (NLSE) by studying the class of equations of the type

$$iz_t + z_{xx} = f(z,z^*), \tag{1.1}$$

where $f(z,z^*)$ is, *a priori*, any complex function. Using a given generalized Pfaffian (exterior differential) system to which this equation is equivalent, we seek by the standard methods[1–8] the possible forms of $f(z,z^*)$ which allow for pseudopotentials satisfying the appropriate integrability conditions. Making the usual assumptions concerning which variables the pseudopotential equation may involve, and requiring that, in particular, pseudopotentials of one complex dimension exist, we find that the permissible $f(z,z^*)$ are very limited. In fact, up to changes in the dependent and independent variables, the only $f(z,z^*)$ for which genuine pseudopotentials exist are the usual expression $f = \epsilon|z|^2 z$ in the standard nonlinear Schrödinger equation and two slightly different ones of the form $f = (\epsilon|z|^2 + b)(z + cz^*)$ and $f = |z|^2(-\epsilon z + z^*) + \epsilon az - a^*z^*$, where the constant a is complex, b and c are real with $c \neq 0$, $\epsilon = \pm 1$. Besides this, we find a list of equations for which the pseudopotential becomes dependent on the original variables (z,z^*,x,t) only; that is, where the resulting integrability equations ar actually equivalent to conservation laws. As a matter of terminology we shall refer to all transformations defining one-dimensional pseudopotentials which are not trivially equivalent to conservation laws as "Bäcklund Transformations" (BT) whether the new variable satisfies the same equation or not. We then show how Lie symmetries in the standard NLSE give rise to the known complex parameter. For the other cases above, no parameter arises.

In Sec. II we replace the NLSE (1.1) by a closed Pfaffian system, introduce the pseudopotentials $y^\mu(x,t)$ and reduce the compatability conditions for the pseudopotentials to a set of commutation relations for certain differential operators. In Sec. III we solve these commutation relations under

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the assumption that all operators involved lie in the algebra sl (2,$\mathbb{C}$). We show that eight different nontrivial cases occur, i.e., eight different types of interaction terms $f(z,z^*)$ for which pseudopotentials exist. For each of them we obtain the pseudopotentials explicitly. In Sec. IV we discuss all the cases obtained in Sec. III. For each interaction we find the linear Lie symmetries of the corresponding NLSE, write down the conservation laws corresponding to the first five pseudopotentials, and the Bäcklund transformations and inverse scattering equations corresponding to the last three. Section V is devoted to conclusions.

II. THE DIFFERENTIAL IDEAL

The nonlinear Schrödinger equation (1.1) is equivalently represented by the following closed Pfaffian system:

$$\begin{aligned}
\omega^1 &= dz\wedge dt - z_x dx\wedge dt,\\
\omega^2 &= i dz\wedge dx - dz_x\wedge dt + f dx\wedge dt,\\
\omega^{1*} &= dz^*\wedge dt - z_x^* dx\wedge dt,\\
\omega^{2*} &= -i dz^*\wedge dx - dz_x^*\wedge dt + f^* dx\wedge dt
\end{aligned}\tag{2.1}$$

(the asterisks denote complex conjugation).

The space on which the 2-forms are defined is (at least locally) the first jet space $J^1(\mathbb{R}^2,\mathbb{C})$ with coordinates (x,t,z,z_x,z_t). We now introduce a mapping

$$\psi: J^1(\mathbb{R}^2,\mathbb{C})\times\mathbb{C}^n \to J^1(\mathbb{R}^2,\mathbb{C}^n),$$

preserving the natural projections onto $\mathbb{R}^2\times\mathbb{C}^n$, expressed in local coordinates by

$$\begin{aligned}
y_x^\mu &= \psi_x^\mu(z,z^*,z_x z_x^*,z_t,z_t^*,y^\nu),\\
y_t^\mu &= \psi_t^\mu(z,z^*,z_x,z_x^*,z_t z_t^*,y^\nu),\\
\mu,\nu &= 1,2,\dots,n,
\end{aligned}\tag{2.2}$$

where $(x,t,y^\mu,y_x^\mu,y_t^\mu)$ are the local coordinates in $J^1(\mathbb{R}^2,\mathbb{C}^n)$.

Note that for simplicity we have assumed that there is no explicit dependence on x, t, and $y^{\nu*}$ in (2.2)

The contact module in $J^1(\mathbb{R}^2,\mathbb{C}^n)$ is generated by the forms

$$\theta^\mu = dy^\mu - y_x^\mu dx - y_t^\mu dt. \tag{2.3}$$

According to the Wahliquist–Estabrook method[1,2] we now require that the pull-back $\psi^*\theta^\mu$ of (2.3), together with the pull-back of the system (2.1) under the trivial projection $J^1(\mathbb{R}^2,\mathbb{C})\times\mathbb{C}^n \to J^1(\mathbb{R}^2,\mathbb{C})$ generate a differential ideal. That is, writing

$$\psi^*\theta^\mu = dy^\mu - \psi_x^\mu dx - \psi_t^\mu dt,$$

we require that

$$d(\psi^*\theta^\mu) = -d\psi_x^\mu\wedge dx - d\psi_t^\mu\wedge dt,$$

should be *linear* in $(\omega^1,\omega^2,\omega^{1*},\omega^{2*},\psi^*\theta^\mu)$.

This condition is equivalent to the following set of partial differential equations for ψ_x^μ and ψ_t^μ.

$$\frac{\partial\psi_x^\mu}{\partial z_x} = \frac{\partial\psi_x^\mu}{\partial z_x^*} = \frac{\partial\psi_x^\mu}{\partial z_t} = \frac{\partial\psi_x^\mu}{\partial z_t^*} = \frac{\partial\psi_t^\mu}{\partial z_t} = \frac{\partial\psi_t^\mu}{\partial z_t^*} = 0, \tag{2.4a}$$

$$\frac{\partial\psi_x^\mu}{\partial z} + i\frac{\partial\psi_t^\mu}{\partial z_x} = 0,\quad \frac{\partial\psi_x^\mu}{\partial z^*} - i\frac{\partial\psi_t^\mu}{\partial z_x^*} = 0, \tag{2.4b}$$

$$\psi_t^\alpha\frac{\partial\psi_x^\mu}{\partial y^\alpha} - \psi_x^\alpha\frac{\partial\psi_t^\mu}{\partial y^\alpha} - \frac{\partial\psi_t^\mu}{\partial z}z_x - \frac{\partial\psi_t^\mu}{\partial z^*}z_x^* = \frac{\partial\psi_t^\mu}{\partial z_x}f + \frac{\partial\psi_t^\mu}{\partial z_x^*}f^*. \tag{2.4c}$$

Equations (2.4a) and (2.4b) can be solved directly and the result can be substituted into (2.4c). We equate the coefficients of equal powers of z_x and z_x^* in (2.4c) and find that ψ_x^μ and ψ_t^μ of (2.2) can be written in the general form

$$\psi_x^\mu = i[|z|^2Q^\mu(y) + zP^\mu(y) - z^*R^\mu(y) + U^\mu(y)], \tag{2.5a}$$

$$\begin{aligned}\psi_t^\mu = {}&(zz_x^* - z^*z_x)Q^\mu(y) - z_xP^\mu(y) - z_x^*R^\mu(y)\\ &+ i[|z|^2V^\mu(y) - zX^\mu(y) - z^*Y^\mu(y) + S^\mu(y)].\end{aligned} \tag{2.5b}$$

In order that Eqs. (2.4) are satisfied, the functions $Q^\mu(y),P^\mu(y),\dots,S^\mu(y)$ must satisfy certain conditions. These are best expressed by introducing vector fields

$$\hat{Q} = Q^\mu(y)\frac{\partial}{\partial y^\mu},\ \hat{P} = P^\mu(y)\frac{\partial}{\partial y^\mu},\ \dots,\ \hat{S} = S^\mu(y)\frac{\partial}{\partial y^\mu}, \tag{2.6}$$

and

$$\hat{\psi}_x = y_x^\mu\frac{\partial}{\partial y^\mu},\quad \hat{\psi}_t = y_t^\mu\frac{\partial}{\partial y^\mu}. \tag{2.7}$$

Equations (2.2), combined with (2.5) are now equivalent to the following operator relations on the image under the mapping ψ:

$$\hat{\psi}_x = i[|z|^2\hat{Q} + z\hat{P} - z^*\hat{R} + \hat{U}], \tag{2.8a}$$

$$\begin{aligned}\hat{\psi}_t = {}&(zz_x^* - z^*z_x)\hat{Q} - z_x\hat{P} - z_x^*\hat{R}\\ &+ i[|z|^2\hat{V} - z\hat{X} - z^*\hat{Y} + \hat{S}].\end{aligned} \tag{2.8b}$$

For the relations (2.4) to be satisfied (identically in z, z^*, $z_xz_x^*,z_t$, and z_t^*) the vector fields in (2.6) must satisfy the following commutation relations:

$$\hat{V} = [\hat{P},\hat{R}],\ \hat{X} = [\hat{P},\hat{U}],\ \hat{Y} = [\hat{R},\hat{U}], \tag{2.9a}$$

$$[\hat{Q},\hat{P}] = 0,\ [\hat{Q},\hat{R}] = 0,\quad [\hat{Q},\hat{U}] = 0, \tag{2.9b}$$

$$\begin{aligned}&[|z|^2\hat{V} - z\hat{X} - z^*\hat{Y} + \hat{S},\ \ |z|^2\hat{Q} + z\hat{P} - z^*\hat{R} + \hat{U}]\\ &\quad = (z^*\hat{Q} + \hat{P})f + (-z\hat{Q} + \hat{R})f^*,\end{aligned} \tag{2.9c}$$

where $f = f(z,z^*)$ is the function figuring in the nonlinear Schrödinger equation (1.1) (NLSE).

A pseudopotential $y^\mu(x,t)$ for the NLSE is obtained in the form (2.2) from (2.8), whenever a solution of the commutation relations (2.9) exists.

We would at this stage like to point out a connection between equations (2.8) and certain classical results on systems of ordinary differential equations. Lie[23a] proved that the necesarry and sufficient condition for the system

$$\frac{dx^i}{dt} = \eta^i(x^1,\dots,x^n,t),\quad i = 1,\dots,n, \tag{2.10}$$

to have a "fundamental set of solutions" (such that the general solution can be written as a function of the fundamental solutions) is that (2.10) be expressible in the form

$$\frac{dx^i}{dt} = \sum_{a=1}^{r} Z^a(t)\xi_a^i(x)\quad i = 1,\dots,n,\ x = (x^1,\dots,x^n), \tag{2.11}$$

where the functions $\xi^i_a(x)$ are such that the operators

$$\hat{X}_a = \sum_{i=1}^{n} \xi^i_a(x) \frac{\partial}{\partial x^i}, \quad 1 \leqslant a \leqslant r, \tag{2.12}$$

generate a finite-dimensional Lie algebra.

Thus, if we require that the set of operators $\hat{Q},\hat{P},\hat{R}$, and $\hat{U}$ be contained in a finite-dimensional Lie algebra of vector fields, (2.8a) satisfies Lie's criterion. For the cases $n = 1$ or 2 this essentially forces (2.8a) to acquire the form of a Riccati equation or a coupled set of Riccati equations.[24,25] This may be the reason why Riccati equations play an important role in all of soliton physics.

III. SOLUTIONS OF THE COMMUTATION RELATIONS

A. General comments

In order to obtain explicit pseudopotentials we may look for solutions to the commutation relations (2.9), within a finite-dimensional Lie algebra, and then choose representations giving $\hat{Q},\hat{P},...,\hat{S}$ as differential operators in the form (2.6).

In general the "pseudopotentials" y are multicomponent objects $y = \{y^\mu\} = (y^1,...,y^n)$, with $y^\mu \in \mathbb{C}$ ($\mu = 1,...,n$). Relations (2.2) for these pseudopotentials reduce to conservation laws if the variable y does not figure on the right hand (or can be eliminated by a transformation of variables). If the right-hand sides are linear in y, then we obtain equations of the type used in the inverse scattering method. The variables $y(x,t)$ will in general themselves satisfy partial differential equations. For $n = 1$ the equation satisfied by $y(x,t)$ may be the same as satisfied by $z(x,t)$ and (2.2) amounts to an inner Bäcklund transformation. If the equations for y differ from those for x we may have an outer Bäcklund transformation (further conditions must be imposed to make this statement exact).

It is well-known that the only Lie algebras that can be realized by operators of the form

$$X_i = f_i(y) \frac{d}{dy},$$

(i.e., holomorphic vector fields in one complex variable) are sl (2,$\mathbb{C}$) and its subalgebras.[23] While we do not restrict ourselves to the case $n = 1$ we shall limit ourselves to the case when all operators (2.6) do lie in the algebra sl(2,$\mathbb{C}$) and provide the most general solution of (2.9) under this assumption.

From here on we assume that all the operators in (2.6) lie in some vector field representation of sl(2,$\mathbb{C}$).

Choosing a basis of sl(2,$\mathbb{C}$) satisfying

$$[\tau_3,\tau_\pm] = \mp i\tau_\pm, \quad [\tau_+,\tau_-] = -2i\tau_3, \tag{3.1}$$

we shall make use of the following representations.

For $n = 1$, we put

$$\tau_3 = iy\frac{d}{dy}, \quad \tau_+ = \frac{d}{dy}, \quad \tau_- = y^2\frac{d}{dy}, \tag{3.2}$$

and

$$\hat{\psi}_x = y_x\frac{d}{dy}, \quad \hat{\psi}_t = y_t\frac{d}{dy}. \tag{3.3}$$

For $n = 2$, we put

$$\tau_3 = \frac{i}{2}(-u\partial_u + v\partial_v), \quad \tau_+ = -iu\partial_v, \quad \tau_- = -iv\partial_u, \tag{3.4}$$

and

$$\hat{\psi}_x = u_x\partial_u + v_x\partial_v, \quad \hat{\psi}_t = u_t\partial_u + v_t\partial_v. \tag{3.5}$$

We now proceed to solve equations (2.9) in sl(2,$\mathbb{C}$). We are interested in solutions up to coordinate transformations and hence up to equivalence under Lie algebra automorphisms. This equivalence allows us to simplify the expressions for one or more of the operators involved. We recall that an arbitrary nonzero element of sl(2,$\mathbb{C}$) is conjugate under SL(2,$\mathbb{C}$) either to τ_+ or to $\alpha\tau_3$ ($\alpha \in \mathbb{C}$). The results below will always be expressed by quoting just one representative of each equivalence class under automorphisms of the underlying algebra.

The commutation relations (2.9) are in general incompatible. Indeed, nontrivial solutions exist only if the interaction term $f(z,z^*)$ satisfies certain conditions to be obtained below. Whenever such an interaction $f(z,z^*)$ is found, we shall simplify it as much as possible by an affine transformation in the unknown variable

$$z' = \alpha z + \beta, \tag{3.6}$$

where α and β are suitably chosen complex constants.

B. Solutions in sl(2,$\mathbb{C}$) for $\hat{Q} \neq 0$

Since $\hat{R},\hat{P}$ and $\hat{U}$ commute with $\hat{Q}$ and all four lie in sl(2,$\mathbb{C}$) we have

$$\hat{P} = p\hat{Q}, \quad \hat{R} = r\hat{Q}, \quad \hat{U} = u\hat{Q},$$
$$\hat{V} = \hat{X} = \hat{Y} = 0, \quad (p,r,u, \in \mathbb{C}), \tag{3.7}$$

and (2.9c) implies

$$(zz^* + zp - z^*r + u)[\hat{S},\hat{Q}] = [(z^* + p)f - (z - r)f^*]\hat{Q}, \tag{3.8}$$

and hence

$$[\hat{S},\hat{Q}] = ik\hat{Q}, \quad k \in \mathbb{C}, \quad \hat{Q} = \tau_+, \quad \hat{S} = -k\tau_3. \tag{3.9}$$

Two possibilities occur.

A. $r = -p^*$, $k = k^*$

Taking $z \to z - p^*$ and redefining the constant u, we have

$$f_1(z,z^*) = \{g(z,z^*) + (ik/2)(1 + u/|z|^2)\}z, \tag{3.10a}$$
$$g(z,z^*) = g^*(z,z^*),$$
$$\hat{\psi}_x = i(|z|^2 + u)\tau_+,$$
$$\hat{\psi}_t = (-z_x z^* + zz^*_x + is)\tau_+ - ik\tau_3. \tag{3.10b}$$

If $k = 0$, then $u, s \in \mathbb{C}$; if $k \neq 0$, then $u \in \mathbb{R}$, $s = 0$.

B. $r \neq -p^*$

We take $z \to \frac{1}{2}(r + p^*)z + \frac{1}{2}(r - p^*)$ and find

$$f_2(z,z^*) = [i/2(z + z^*)] \times \{k(|z|^2 + z - z^* + u)(z + 1) - k^*(|z|^2 - z + z^* + u^*)(z - 1)\}, \tag{3.11a}$$
$$\hat{\psi}_x = i(|z|^2 + z - z^* + u)\tau_+,$$
$$\hat{\psi}_t = [-z_x(z^* + 1) - z^*_x(z - 1)]\tau_+ - ik\tau_3. \tag{3.11b}$$

Notice that f_1 involves an arbitrary real function $g(z,z^*)$, f_2 involves only free constants. The function $g(z,z^*)$ does not figure in (3.10b). We shall show in Sec. IV that the obtained pseudopotentials simply provide conservation laws.

C. Solutions in sl(2,$\mathbb{C}$) for $\hat{Q}=0$

Relations (2.9b) are satisfied trivially. We separately consider the cases when $\hat{R}=\alpha\hat{P}$ and $\hat{R}\neq\alpha\hat{P}$.

A. $\hat{R}=\alpha\hat{P}$, $\alpha\in\mathbb{C}$, $\alpha\neq 0$

We now consider individual SL(2,$\mathbb{C}$) orbits of $\hat{P}$.

A1: $\hat{P}=p\tau_3$, $\quad \hat{R}=r\tau_3$, $\quad pr\neq 0$.

The algebra (2.9) can only be solved if $f(z,z^*)=|f(z,z^*)|e^{i\phi}$ where ϕ is a *constant* phase. Taking $z\to ze^{-i\phi}$ we obtain

$$f_3(z,z^*)=f_3^*(z,z^*), \tag{3.12a}$$

$$\hat{\psi}_x=i[p(z+z^*)+u]\tau_3, \tag{3.12b}$$

$$\hat{\psi}_t=[p(-z_x+z_x^*-s]\tau_3$$

[i.e., $f_3(z,z^*)$ is an arbitrary real function].

A2: $\hat{P}=p\tau_+$, $\quad \hat{R}=r\tau_+$, $\quad pr\neq 0$, $\quad |p|=|r|$.

We can transform z and conjugate in sl(2,$\mathbb{C}$) to set $p=-r=1$. This gives

$$f_4(z,z^*)=g(z,z^*)+az, \tag{3.13a}$$

$$g(z,z^*)=g^*(z,z^*),$$

$$\hat{\psi}_x=i(z+z^*)\tau_++iu\tau_3,\quad u^2=\mathrm{Re}a,$$

$$\hat{\psi}_t=[-z_x+z_x^*+u(z-z^*)]\tau_++is\tau_3,\quad s=-\mathrm{Im}a. \tag{3.13b}$$

A3: $\hat{P}=p\tau_+$, $\quad \hat{R}=r\tau_+$, $\quad pr\neq 0$, $\quad |p|\neq|r|$.

By SL(2,$\mathbb{C}$) conjugation we can choose $rp=1$ and obtain

$$f_5(z,z^*)=Az+Bz^*+C. \tag{3.14a}$$

For $|A|^2-|B|^2\neq 0$ we can transform z so that $C=0$, $B=B^*$. For $|A|^2-|B|^2=0$ we can transform so that $A=B$, $C=\epsilon C^*$ ($\epsilon=1$ if $\mathrm{Im}A\neq 0$, $\epsilon=-1$ if $\mathrm{Im}A=0$, $\mathrm{Re}A\neq 0$).

For $C=0$ and $B=B^*$ we define

$$s=(i/2p^2)[p(A-A^*)-(p^4-1)B],$$

$$u^2=(1/2p^2)[p^2(A+A^+)+(p^4-1)B],\quad u_+=0.$$

For $A=B\neq 0$, $C=\epsilon C^*$ we define

$$s=\frac{i(1-p^2)}{2p^2}(p^2A+A^*),$$

$$u^2=\frac{1+p^2}{2p^2}(p^2A+A^*),\quad u_+=\frac{2p(p^2+\epsilon)}{1-p^2}\frac{C}{p^2A+A^*}.$$

In both cases, the pseudopotentials satisfy

$$\hat{\psi}_x=i[pz-(1/p)z^*+u_+]\tau_++iu\tau_3,$$

$$\hat{\psi}_t=p(uz-z_x)+(1/p)(uz^*-z_x^*)+is\tau_3. \tag{3.14b}$$

Notice that p is a free parameter, s, u, and u_+ are given in terms of A, B, C, and p.

A4: $\hat{P}=\hat{R}=0$.

The function $f(z,z^*)$ is arbitrary, the Bäcklund transformation (BT) trivial.

B. *$\hat{R}$ and $\hat{P}$ linearly independent*

In this case (2.9c) implies that $f(z,z^*)$ can be written as

$$f(z,z^*)=g_1z^2z^*+g_2zz^{*2}+g_3z^2+g_4z^{*2}+g_5zz^*+g_6z+g_7z^*+g_8,$$

$$g_i\in\mathbb{C}, \tag{3.15}$$

satisfying

$$[\hat{V},\hat{P}]=g_1\hat{P}+g_2^*\hat{R},\quad 2[\hat{V},\hat{U}]=g_5\hat{P}+g_5^*\hat{R},$$

$$[\hat{V},\hat{R}]=-g_2\hat{P}-g_1^*\hat{R},$$

$$[\hat{X},\hat{U}]-[\hat{S},\hat{P}]=-g_6\hat{P}-g_7^*\hat{R}, \tag{3.16}$$

$$[\hat{X},\hat{P}]=-g_3\hat{P}-g_4^*\hat{R},$$

$$[\hat{Y},\hat{U}]+[\hat{S},\hat{R}]=-g_7\hat{P}-g_6^*\hat{R},$$

$$[\hat{Y},\hat{R}]=g_4\hat{P}+g_3^*\hat{R},\quad [\hat{S},\hat{U}]=g_8\hat{P}+g_8^*\hat{R}.$$

We proceed further by transforming $\hat{P}$ into $p\tau_3$, τ_+, or 0 and then using the stabilizer of $\hat{P}$ in SL(2,$\mathbb{C}$) to simplify $\hat{R}$. We then solve the commutation relations (2.9a) and (3.16), find the g_i in (3.15), and simplify using (3.6).

Let us discuss the individual cases.

B1: $\hat{P}=p\tau_3$, $\quad \hat{R}=\tau_++r\tau_3$, $\quad p\neq 0$

$$f_6(z,z^*)=|z|^2(-\epsilon z+z^*)+\epsilon az-a^*z^*,\quad \epsilon=\pm 1,$$

$$\hat{\psi}_x=i(z-\epsilon z^*)\tau_3-iz^*\tau_+, \tag{3.17a}$$

$$\hat{\psi}_t=-[z_x+\epsilon z_x^*+\epsilon(a-a^*)]\tau_3+(-z_x^*+|z|^2-a)\tau_+. \tag{3.17b}$$

B2: $\hat{P}=p\tau_3$, $\quad \hat{R}=r(\tau_++\tau_-)+r_3\tau_3$, $\quad rp\neq 0$

$$f_7(z,z^*)=(\epsilon|z|^2+B)(z+Cz^*),\quad \epsilon=\pm 1$$

$$r=[(p^4-1)^{1/4}]/2p,\quad r_3=-\epsilon/p,$$

$$C=\epsilon p^2,\quad B=B^*,\quad p=p^*, \tag{3.18a}$$

$$\hat{\psi}_x=i[pz+(\epsilon/p)z^*]\tau_3-(iz^*/2p)(p^4-1)^{1/2}(\tau_++\tau_-),$$

$$\hat{\psi}_t=[-pz_x+(\epsilon/p)z_x^*]\tau_3-[(p^4-1)^{1/2}/2p]z_x^*(\tau_++\tau_-)+\tfrac{1}{2}[|z|^2+B](p^4-1)^{1/2}(\tau_+-\tau_-). \tag{3.18b}$$

Notice that contrary to all previous cases, the entire sl(2,$\mathbb{C}$) is involved in (3.18b) (τ_+, τ_-, and τ_3 all figure).

B3: $\hat{P}=p\tau_3$, $\quad \hat{R}=0$, $\quad p\neq 0$.

The only solution is $f(z,z^*)=0$.

B4: $\hat{P}=0$, $\quad \hat{R}\neq 0$.

This leads only to $f(z,z^*)=az+b$, ($a,b,\in\mathbb{C}$). The equation is linear and we shall not give the pseudopotential which is of little interest.

B5: $\hat{P}=\tau_+$, $\quad \hat{R}=0$.

Again $f(z,z^*)=az+b$.

B6: $\hat{P}=\tau_+$, $\quad \hat{R}\neq 0$.

Performing an $\exp(\alpha\tau_+)$ transformation, we can transform $\hat{R}$ to the form $\hat{R}=r_-\tau_-+r_3\tau_3$. The relations for $[\hat{V},\hat{P}]$ and $[\hat{V},\hat{R}]$ imply $r_3=0$. Thus $\hat{R}=r\tau_-$. We obtain, after simplification,

$$f_8(z,z^*)=(\epsilon/2)|z|^2+bz,\quad b=b^*, \tag{3.19a}$$

and

$$\hat{\psi}_x = i[z\tau_+ + z^*(\epsilon/4)\tau_- + u\tau_3],$$
$$\hat{\psi}_t = (-z_x + uz)\tau_+ + (\epsilon/4)(z_x^* + uz^*)\tau_- + [-(\epsilon/2)|z|^2 + u^2 - b]\tau_3. \quad (3.19b)$$

For $b = 0$ this case reduces to the usual "nonlinear Schrödinger equation" (cubic Schrödinger equation).

IV. SYMMETRIES, CONSERVATION LAWS, AND BÄCKLUND TRANSFORMATIONS

In Sec. III we have found eight different forms of the interaction terms $f(z,z^*)$ in the nonlinear Schrödinger equation (1.1), for which pseudopotentials exist.

In this section we shall discuss the individual cases, and obtain the Lie symmetries of the equations, the conservation laws and inverse scattering equations.

A. Lie symmetries for the NLSE

To study the symmetries of the equations considered above, we may proceed by a number of different methods. The most familiar approach[23,14] consists of applying finite or infinitesimal transformations in the space of dependent and independent variables, and requiring that these map solutions of the equation into solutions. An alternative approach, which is closer in spirit to the computation of the previous sections, consists of determining the symmetries of the differential ideal. Again, a finite or infinitesimal approach may be taken. The latter[26,27] is what will be described here although the same results are obtained by the direct study of the infinitesimal invariances of the equations themselves. The finite transformations may subsequently be determined by integration.

The infinitesimal symmetries are vector fields $\widetilde{X}$ on the jet space $J^1(R^2,\mathbb{C})$ with coordinates (x,t,z,z_x,z_t) for which the Lie derivatives of the generators (2.1) of the differential ideal remain in the ideal:

$$\mathscr{L}_{\widetilde{X}}\omega^1 = a_1^1\omega^1 + a_2^1\omega^2 + b_1^1\omega^{1} + b_2^1\omega^{2}, \quad (4.1a)$$

$$\mathscr{L}_{\widetilde{X}}\omega^2 = a_1^2\omega^1 + a_2^2\omega^2 + b_1^2\omega^{1} + b_2^2\omega^{2} \quad (4.1b)$$

(plus the complex conjugate relations). The general form of $\widetilde{X}$ is

$$\widetilde{X} = a(x,t)\frac{\partial}{\partial t} + b(x,t)\frac{\partial}{\partial x} + c(x,t,z,z^*)\frac{\partial}{\partial z} + c^*(x,t,z,z^*)\frac{\partial}{\partial z^*} + e(x,t,z,z_x,z_x^*,z_t,z_t^*)\frac{\partial}{\partial z_x} + e^*(x,t,z,z_x,z_x^*,z_t,z_t^*)\frac{\partial}{\partial z_x^*}. \quad (4.2)$$

There are no $\partial/\partial z_t$ or $\partial/\partial z_t^*$ terms since it is sufficient to work on the partial jet space $\{x,t,z,z^*,z_x,z_x^*\}$ in view of the expressions (2.1) defining $\{\omega^1,\omega^2,\omega^{1*},\omega^{2*}\}$. In fact, the detailed form of $e(x,t,z,\cdots)$ is determined from the coefficients a, b, c [see Eq. (4.5)], since we are dealing here with a prolongation of a vector field on the space $J^\circ(R^2,\mathbb{C})$ that is, with an infinitesimal Lie transformation.

The corresponding transformation acting upon sections of $J^\circ(R^2,\mathbb{C})$, that is, functions $z(x,t)$, is given by the operator

$$X = a(x,t)\frac{\partial}{\partial t} + b(x,t)\frac{\partial}{\partial x} - c(x,t,z,z^*), \quad (4.3)$$

and hence $e^{\alpha X}z(x,t)$ is a solution of Eq. (1.1) whenever $z(x,t)$ is. The fact that $\widetilde{X}$ is the prolongation of a Lie transformation need not be assumed *a priori*, but is assured by the presence of the forms $\{\omega^1,\omega^{1*}\}$ in the ideal. We simplify matters however by allowing a and b to depend only upon the independent variables (x,t) and c only on (x,t,z,z^*) at the beginning. It follows from (4.1) that $c(x,t,z,z^*)$ is at most linear inhomogeneous in z and z^*. We shall simplify further by taking it to be of the form

$$c(x,t,z,z^*) = c(x,t)z, \quad (4.4)$$

that is, purely linear in z.

Equation (4.1a) implies that

$$a_x = 0, \quad (4.5a)$$

and

$$e = c_x z + cz_x - b_x z_x. \quad (4.5b)$$

Equation (4.1b) implies

$$a_t = 2b_x, \quad \text{and} \quad ib_t = 2c_x, \quad (4.6)$$

as well as

$$(c - 2b_x)f - czf_z - c^*z^*f_{z^*} + (ic_t + c_{xx})z = 0. \quad (4.7)$$

Integrating (4.5a) and (4.6) shows a, b, and c to be of the form

$$a(x,t) = \alpha(t),$$
$$b(x,t) = \frac{\alpha'(t)}{2}x + \beta(t),$$
$$c(x,t) = i\left[\frac{\alpha''(t)}{2}x^2 + \frac{\beta'(t)}{2}x + \gamma(t)\right]. \quad (4.8)$$

Substituting in (4.7) and equating like powers of x gives

$$i\alpha''[f - zf_z + z^*f_{z^*}] = \alpha'''z,$$
$$i\beta'[f - zf_z + z^*f_{z^*}] = \beta''z,$$
$$i[(\gamma - i\alpha')f - \gamma zf_z + \gamma^*z^*f_{z^*}] = (\gamma' - (i/4)\alpha'')z. \quad (4.9)$$

It is easy to see that $\gamma(t) = 0, \alpha'(t) = 0, \beta'(t) = 0$ is a solution for any $f(z,z^*)$. Thus, translational invariance is always present: $X = P$ and $X = H$ satisfy (4.5) for any interaction $f(z,z^*)$, where

$$P = \frac{\partial}{\partial x}, \quad H = \frac{\partial}{\partial t}. \quad (4.10)$$

This is, of course, a trivial expression of the fact that the coefficients in the NLSE do not depend explicitly on x and t.

We stress that the use of the infinitesimal operator X satisfying (4.3), (4.4) is a definite restriction. For the free-particle Schrödinger equation (1.1) with $f(z,z^*) = 0$ this approach would lead to the Schrödinger group Sch(1) and its Lie algebra[14,28]

$$H = \partial_t, \quad D = 2t\partial_t + x\partial_x + \lambda,$$
$$C = t^2\partial_t + tx\partial_x + t/2 - ix^2/4, \quad (4.11)$$
$$P = \partial_x, \quad B = -t\partial_x + ix/2,$$
$$E_1 = i, \quad E_2 = 1 \quad (\lambda\in\mathbb{C}).$$

A consideration of more general transformations than linear ones would clearly be desirable in the context of nonlinear partial differential equations.[21,29–32]

Here D, C, and B correspond to dilations, conformal transformations, and Galilei "boosts," respectively, H and P to translations, and E_1 and E_2 to multiplication, of z by an arbitrary constant.

Now let us consider individual cases obtained in Sec. III.

B. Discussion of pseudopotentials leading to conservation laws

$$f_1(z,z^*): z_{xx} + iz_t = [g(z,z^*) + (ik/2)(1 + u/|z|^2)]z, \tag{4.12a}$$

$$g(z,z^*) = g^*(z,z^*).$$

The only solution of (4.9) valid for all $g(z,z^*)$ is $\alpha' = \beta' = \gamma = 0$ so that the only Lie symmetries are translations. The pseudopotential defined by (3.10b) however provides a conservation law. Using (3.2) and (3.3), we have

$$y_x = i(|z|^2 + u),$$
$$y_t = (-z_x z^* + zz_x^*) + ky. \tag{4.12b}$$

Putting $\tilde{y}(x,t) = e^{-kt}y(x,t)$, substituting into (4.12b), and setting $(\tilde{y}_x)_t = (\tilde{y}_t)_x$, we obtain the "time-dependent" conservation law

$$i\frac{\partial}{\partial t}[(|z|^2 + u)e^{-kt}] + \frac{\partial}{\partial x}[(z_x z^* - zz_x^*)e^{-kt}] = 0. \tag{4.12c}$$

If appropriate asymptotic conditions are satisfied and $u \leqslant 0$ there will be a conserved quantity

$$w(k) = \int_{-\infty}^{\infty} [(|z|^2 + u)e^{-kt}]dx. \tag{4.12d}$$

(For $k = 0$ this quantity can be interpreted as the total probability.)

$f_2(z,z^*)$:

$$z_{xx} + iz_t = [i/2(z + z^*)]\{k(zz^* + z - z^* + u)(z + 1) - k^*(zz^* - z + z^* + u^*)(z - 1)\}. \tag{4.13a}$$

Equation (4.9) allows for a nontranslational symmetry in this case only if $u = 0$, $k = k^*$. Then

$$z_{xx} + iz_t = ikz^2/(z + z^*), \tag{4.13b}$$

and the symmetries are

$$P = \frac{\partial}{\partial x}, \quad H = \frac{\partial}{\partial t}, \quad E = 1, \tag{4.13c}$$

where E indicates that z in (4.13b) can be multiplied by a real constant.

Equations (3.11b) always provide a conservation law. Proceeding as in case (4.12) we have

$$i\frac{\partial}{\partial t}[(|z|^2 + z - z^* + u)e^{-kt}] + \frac{\partial}{\partial x}[z_x(z^* + 1) - z_x^*(z - 1)e^{-kt}] = 0. \tag{4.13d}$$

$$f_3(z,z^*): z_{xx} + iz_t = f(z,z^*), \quad f(z,z^*) = f^*(z,z^*). \tag{4.14a}$$

There are no nontranslational symmetries but (3.12b) provides a conservation law

$$i\frac{\partial}{\partial t}(z + z^*) + \frac{\partial}{\partial x}(z_x - z_x^*) = 0. \tag{4.14b}$$

$$f_4(z,z^*): z_{xx} + iz_t = g(z,z^*) + az^*. \tag{4.15a}$$

Again, in general there are no nontranslational symmetries. Equation (3.13b) can be rewritten by putting $w = e^{ux+st}y$ and using (3.2) and (3.3). The obtained conservation law $(w_x)_t = (w_t)_x$ is

$$i\frac{\partial}{\partial t}[(z + z^*)e^{ux+st}] + \frac{\partial}{\partial x}\{[z_x - z_x^* - u(z - z^*)]e^{ux+st}\} = 0. \tag{4.15b}$$

$$f_5(z,z^*): z_{xx} + iz_t = Az + Bz^* + C. \tag{4.16a}$$

Nontranslational symmetries only exist in special cases, namely the following

(i) $A = B = 0$, $C \neq 0$. Dilation symmetry:

$$P, H, \text{ and } D = 2t\partial_t + x\partial_x - 2, \quad z'(x,t) = a^{-2}z(ax,a^2t). \tag{4.16b}$$

(ii) $C = 0$, $B \neq 0$. Multiplication by a real constant:

$$P, H, \text{ and } E = 1, \quad z'(x,t) = az(x,t), \quad a = a^*. \tag{4.16c}$$

(iii) $B = C = 0$, $A \neq 0$. Symmetry under the Schrödinger group Sch(1). In addition to

$$P = \frac{\partial}{\partial x}, \quad H = \frac{\partial}{\partial t}, \quad E_1 = i, \quad \text{and} \quad E_2 = 1, \tag{4.16d}$$

i.e., $z'(x,t) = \alpha z(x + x_0, t + t_0)$, we have Galilei invariance

$$B = -t\partial_x + (i/2)x,$$
$$z'(x,t) = \exp[(ib/2)(x - bt/2)]z(x - bt,t), \tag{4.16e}$$

a modified dilation invariance

$$D = 2t\partial_t + x\partial_x + 2iAt,$$
$$z'(x,t) = \exp[-iA(1 - a^2)t]z(ax,a^2t), \tag{4.16f}$$

and a modified conformal invariance

$$C = t^2\partial_t + tx\partial_x + (\tfrac{1}{2}t - \tfrac{1}{4}ix^2 + iAt^2),$$
$$z'(x,t) = (1 + ct)^{-1/2}\exp\left[\frac{ic}{4(1 + ct)}(x^2 - 4At^2)\right] \times z\left(\frac{x}{1 + ct}, \frac{t}{1 + ct}\right). \tag{4.16g}$$

These symmetries for the linear Schrödinger equation $z_{xx} + iz_t = Az$ have been studied elsewhere.[28] Putting

$$w(x,t) = e^{ux+st}y(x,t),$$

we obtain a conservation law from Eq. (3.14b) valid for arbitrary A, B, and C and hence independent of the above linear Lie symmetries

$$i\frac{\partial}{\partial t}\left[e^{ux+st}(pz - \frac{1}{p}z^* + u_+)\right] + \frac{\partial}{\partial x}\left[e^{ux+st}\{p(z_x - uz) + \frac{1}{p}(z_x^* - uz^*)\}\right] = 0. \tag{4.16h}$$

Let us summarize the results of this section.

(1) The interactions $f_1(z,z^*),\ldots,f_5(z,z^*)$ all allow for potentials y that provide conservation laws for the correspond-

ing Schrödinger equation.

(2) The interactions f_1, f_3, and f_4 each involve an arbitrary real function which does not figure in the pseudopotential equations.

(3) The algebras leading to these cases were one or two dimensional subalgebras of sl(2,$\mathbb{C}$).

(4) In general the conservation laws are not related to the linear Lie symmetries of the considered equation.

The remaining three interactions f_6, f_7, and f_8 are somewhat different.

C. Discussion of pseudopotentials leading to Bäcklund transformations and to inverse scattering equations

$$f_6(z,z^*): z_{xx} + iz_t = |z|^2(-\epsilon z + z^*) + \epsilon az - a^*z^*. \tag{4.17a}$$

Using the one-variable realization (3.2) and (3.3) we rewrite the transformation (3.17b) as

$$\begin{aligned} y_x &= -(z - \epsilon z^*)y - iz^*, \\ y_t &= -i[z_x + \epsilon z_x^* + \epsilon(a - a^*)]y + (-z_x^* + |z|^2 - a). \end{aligned} \tag{4.17b}$$

The equations (3.17b) involve a two-dimensional subalgebra of sl(2,$\mathbb{C}$) with basis (τ_3,τ_+). Contrary to previous cases, the terms in (4.17b) involving y also depend on z. Hence (4.17b) cannot be reduced to a conservation law by a simple transformation of the y variable alone.

In general (4.17a) has only translational symmetries. For $a = 0$ we also have dilation invariance

$$D = 2t\partial_t + x\partial_x + 1, \tag{4.17c}$$

$$z'(x,t) = [e^{bD}z](x,t) = bz(bx,b^2t), \quad b = b^*.$$

Notice that (4.17b) does not involve a free parameter [both a and ϵ figure in $f_6(z,z^*)$]. If we write (4.17b) for $a = 0$ and perform the dilation (4.17c), no parameter is introduced.

Equations (4.17b) represent an outer Bäcklund transformation. The new variable y satisfies an evolution equation that can be obtained by solving for z and z^* from the first of equations (4.17b) and its complex conjugate and substituting the result into the second equation. The resulting equation for y is nonlinear and complicated and we shall not reproduce it here.

Outer Bäcklund transformations can in some cases be transformed into inner ones by making use of the symmetries of the equations involved. For Eq. (4.17a) however, this is not possible. Indeed, assume that a function $u(x,t)$ exists, that satisfies Eq. (4.17a) whenever $z(x,t)$ satisfies this equation and y satisfies (4.17b). We put $u(x,t) = F(z,z^*,y,y^*)$ and then substitute u and u^* into (4.17a) and its complex conjugate. Requiring that the obtained pde for F be an identity in z,z^*, and their derivatives whenever (4.17a) is satisfied, we find that no such function F exists, other than z itself.

The BT (4.17b) has a form reminiscent of the inverse scattering equations,[33–37] that have been most successfully applied to solve certain nonlinear pde. Equations (4.17b) are linear in y, involving z as a "potential." The second equation gives the time development of y, the first one describes the "scattering." These equations, however, contain no free parameter that could serve as an eigenvalue for the problem.

A conservation law for the NLSE (4.17a) can be derived directly from the equation [by adding ϵ times the complex conjugate equation to (4.17a)]. We obtain

$$i\frac{\partial}{\partial t}(z - \epsilon z^*) + \frac{\partial}{\partial x}(z_x + \epsilon z_x^*) = 0. \tag{4.17d}$$

A conserved quantity can also be derived from the BT (4.17b). Indeed put

$$\tilde{y}(x,t) = y \exp[\textstyle\int_0^x(z - \epsilon z^*)dx'].$$

Then

$$\tilde{y}_x = -iz^* \exp[\textstyle\int_0^x(z - \epsilon z^*)dx'],$$

so that $\tilde{y}_x$ is expressed in terms of z and z^* alone. Since (4.17b) are compatible when z satisfies (4.17a) we must have $(y_x)_t = (y_t)_x$. Hence

$$\begin{aligned} I = &\textstyle\int_{-\infty}^{\infty} z^*(x,t) \\ &\times (\exp\{\textstyle\int_0^x[z(x',t) - \epsilon z^*(x',t)]dx'\})dx, \end{aligned} \tag{4.17e}$$

must, if it exists, i.e., if the integral converges, be a conserved quantity.

$$f_7(z,z^*): z_{xx} + iz_t = (\epsilon|z|^2 + B)(z + Cz^*), \tag{4.18a}$$

$$\epsilon = \pm 1, \quad B = B^*, \quad C = C^* = \epsilon p^2 \neq 0.$$

The algebra underlying (3.18b) is all of sl(2,$\mathbb{C}$) and the BT involves no free parameters. Using the one-variable realization (3.2) of sl(2,$\mathbb{C}$), we rewrite the BT (3.18b) as

$$\begin{aligned} y_x &= -(pz + \frac{\epsilon}{p}z^*)y - iz^* \frac{(p^4 - 1)^{1/2}}{2p}(1 + y^2), \\ y_t &= -i(z_xp - z_x^*\frac{\epsilon}{p})y - z_x^* \frac{(p^4 - 1)^{1/2}}{2p}(1 + y^2) \\ &\quad + \tfrac{1}{2}[|z|^2 + B](p^4 - 1)^{1/2}(1 - y^2). \end{aligned} \tag{4.18b}$$

Let us first discuss the Lie symmetries of Eqs. (4.18a). If $B \neq 0$ Eq. (4.9) implies that Eq. (4.18a) allows for translational invariance only. For $B = 0$ we also have dilation invariance

$$D = 2t\partial_t + x\partial_x + 1, \quad z'(x,t) = az(ax,a^2t). \tag{4.18c}$$

If we define that under dilations y transforms as $y' = y(ax,a^2t)$ then we can easily check that y' and z' are related by the same BT as y and z. Thus, the dilations do not introduce a parameter into the Bäcklund transformations (4.18b).

The BT (4.18b) is an outer one. The new variable $y(x,t)$ satisfies a complicated nonlinear evolution equation. We obtain it by first solving the first of Eqs. (4.18b), together with its complex conjugate, for z and z^*, then calculating z_x and z_x^* and substituting into the second of Eqs. (4.18b). We have attempted to obtain an inner Bäcklund transformation for Eq. (4.18a) from (4.18b) by setting $u = F(z,z^*,y,y^*)$ and requiring that u satisfy (4.18a) when z satisfies this equation and y satisfies (4.18b). However no such function $F(z,z^*,y,y^*)$ exists, other than z itself.

Finally, let us obtain linear equations of the type used in the inverse scattering method for the NLSE (4.18a). Substituting the two-variable representation (3.4) and (3.5) for τ_i into (3.18b) we obtain

$$\begin{pmatrix} u_x \\ v_x \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(pz - r_3 z^*) & -rz^* \\ -rz^* & -\frac{1}{2}(pz - r_3 z^*) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \qquad (4.18\text{d})$$

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \frac{1}{2}i(z_x p + z_x^* r_3) & iz_x^* r + i(|z|^2 pr - s) \\ iz_x^* r - i(|z|^2 pr - s) & -\frac{1}{2}i(z_x p + z_x^* r_3) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \qquad (4.18\text{e})$$

As required, these equations are linear in u and v and should be compared to those of the Zakharov–Shabat and Ablowitz–Kaup–Newell–Segur approaches. However, the lack of a free parameter in the BT implies that there is no eigenvalue in (4.18d), so the standard techniques cannot be directly applied.

$$f_8(z,z^*): z_{xx} + iz_t = (\epsilon/2)|z|^2 z + bz, \quad b = b^*, \quad \epsilon = \pm 1. \qquad (4.19\text{a})$$

As mentioned above, for $b = 0$ this is the much studied standard "nonlinear Schrödinger equation".[2,33–36,38–47] The case $b \neq 0$ can be transformed into the $b = 0$ case by the time-dependent change of dependent variable $z(x,t) \to e^{ibt} z(x,t)$. We shall hence consider $b = 0$ in (4.19a) and discuss the equation

$$z_{xx} + iz_t = (\epsilon/2)|z|^2 z. \qquad (4.19\text{b})$$

The BT for this case were obtained by Wahlquist and Estabrook.[2] In order to obtain their formulas, we must use a slightly modified realization of sl(2,ℂ), namely

$$\tau_+ = \frac{i}{2} y^2 \frac{d}{dy}, \quad \tau_- = -2i \frac{d}{dy}, \quad \tau_3 = -iy \frac{d}{dy},$$

and put $u = k$ in (3.19b). We obtain

$$y_x = -\tfrac{1}{2}(zy^2 - \epsilon z^* + 2ky),$$
$$y_t = -\tfrac{1}{2}ik(zy^2 - \epsilon z^* + 2ky) + \tfrac{1}{2}i(-z_x y^2 - \epsilon z_x^* + \epsilon |z|^2 y). \qquad (4.19\text{c})$$

The NLSE (4.19b) has a large invariance group, namely a five-dimensional subgroup of the Schrödinger group Sch(1). A basis for its Lie algebra is

$$H = \frac{\partial}{\partial t}, \quad P = \frac{\partial}{\partial x}, \quad E = i$$
$$B = -t \frac{\partial}{\partial x} + \frac{ix}{2}, \quad D = 2t \frac{\partial}{\partial t} + x \frac{\partial}{\partial x} + 1. \qquad (4.19\text{d})$$

The operators B and D generate Galilei transformations (boosts) and dilations respectively, and they are together responsible for the complex parameter k in (4.19c). To see this we write Eqs. (4.19c) for, e.g., $k = 1$:

$$\tilde{y}_x = -\tfrac{1}{2}(\tilde{z}\tilde{y}^2 - \epsilon \tilde{z}^* + 2\tilde{y}),$$
$$\tilde{y}_t = -\tfrac{1}{2}ik(\tilde{z}\tilde{y}^2 - \epsilon \tilde{z}^* + 2\tilde{y}) + \tfrac{1}{2}i(-\tilde{z}_x \tilde{y}^2 - \epsilon \tilde{z}_x^* + \epsilon |\tilde{z}|^2 \tilde{y}).$$

Putting

$$\tilde{z}(x,t) = a e^{ib(x - bt/2)/2} z[a(x - bt), a^2 t],$$
$$\tilde{y}(x,t) = e^{-ib(x - bt/2)/2} y[a(x - bt), a^2 t], \qquad (4.19\text{e})$$

we find that y and z satisfy (4.19c) with

$$k = 1/a - ib/2a \quad (a = a^*, b = b^*). \qquad (4.19\text{f})$$

The BT (4.19c) are outer ones and $y(x,t)$ satisfies a complicated nonlinear evolution equation that can be obtained directly from (4.19c). It is in this case possible to perform a transformation to a new variable $w = F(z,z^*,y,y^*)$ which satisfies Eq. (4.19b). The function w will then be related to z by an inner Bäcklund transformation. To obtain the function $F(z,z^*,y,y^*)$ we evaluate $w_{xx} + iw_t$, use Eq. (4.19b) and its conjugate to eliminate z_{xx} and z_{xx}^* terms, and (4.19c) to eliminate y_{xx}, y_x, and y_t terms. We then require that $w_{xx} + iw_t = (\epsilon/2)w|w|^2$ be satisfied identically in z_t, z_x, z and their complex conjugates. The result is [2,5]

$$w(x,t) = z(x,t) + [2(k + k^*)y^*/(|y|^2 - \epsilon)]. \qquad (4.19\text{g})$$

Thus, if we take a specific solution $z(x,t)$ of (4.19b), substitute it into Eqs. (4.19c), solve for $y(x,t)$ and substitute into (4.19g), we obtain a new solution $w(x,t)$. Lamb[38] has directly obtained an inner Bäcklund transformation for the cubic Schrödinger equation, using a different method.

Again, we can obtain the inverse scattering equations for (3.19b), using the two-variable realization (3.4) and (3.5). Putting $u = -k$ in (3.19b) we have

$$\begin{pmatrix} u_x \\ v_x \end{pmatrix} = \begin{pmatrix} -\frac{1}{2}k & \frac{\epsilon}{4} z^* \\ z & \frac{1}{2}k \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}, \qquad (4.19\text{h})$$

$$\begin{pmatrix} u_t \\ v_t \end{pmatrix} = \begin{pmatrix} \frac{1}{2}i(\frac{1}{2}\epsilon|z|^2 - k^2) & -i\epsilon(z_x^* - kz^*)/4 \\ i(z_x + kz) & -\frac{1}{2}i(\frac{1}{2}\epsilon|z|^2 - k^2) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix},$$

which correspond to the equations used by Zakharov and Shabat.[34]

V. CONCLUSIONS

Having replaced the generalized nonlinear Schrödinger equation $z_{xx} + iz_t = f(z,z^*)$ by a specific Pfaffian system and having made certain assumptions about the forms of the pseudopotentials we have found all functions $f(z,z^*)$ for which such pseudopotentials exist. In addition to the trivial case of a linear interaction $f(z,z^*) = az + b$ we have found eight different classes of such functions $f(z,z^*)$. Five of them lead to pseudopotentials that provide simple conservation laws and conserved quantities that are not obtained from any linear Lie symmetries of the NLSE. The existence of conserved quantities for a pde is of great value in numerical calculations and provides a criterion for the quality of a numerical solution.[47] The three remaining functions $f(z,z^*)$ lead to Bäcklund transformations and to linear equations of the inverse scattering type. Only in the case of the ordinary cubic NLSE does the Bäcklund tranformation involve a free parameter. This free parameter, as we have shown, is due to the combined dilation and Galilei invariance of the equation $z_{xx} + iz_t = \frac{1}{2}\epsilon z|z|^2$ and to the fact that the corresponding BT is not invariant under these two transformations. The free parameter is necessary in order to obtain permutability theorems and the corresponding "nonlinear superposition laws" and also serves as an eigenvalue parameter in the inverse scattering method.

It must be emphasized that the class of nonlinear Schrödinger equations which admit pseudopotentials may be larger than those found here. The assumption in (2.2) on the lack of dependence of ψ on the variables x,t, and $y^{\mu *}$, was made for simplicity only and may be abandoned. The assumption about all vector fields belonging to an sl(2,ℂ) representation was also for convenience. Even in the 1-dimensional case, the underlying algebra might be infinite-dimensional. Furthermore, within the Wahlquist–Estabrook (W–E) approach, the choice of integrable exterior system is crucial. A different choice, which nevertheless has the same maximal integral manifolds, may lead to entirely different pseudopotentials. As an example we might have used the following:

$$\mu^1 = dz - z_t dt - z_x dx, \quad \mu^{1*} = dz^* - z_t^* dt - z_x^* dx,$$
$$\mu^2 = dz_t \wedge dt + dz_x \wedge dx, \quad \mu^{2*} = dz_t^* \wedge dt + dz_x^* \wedge dx, \tag{5.1}$$
$$\mu^3 = dz_x \wedge dt - (f - iz_t) dx \wedge dt.$$

Although the ideal generated by (5.1) has the same maximal integral manifolds as (2.1), it is not identical to it. In fact, the resulting pseudopotentials may involve z_t, unlike those we have studied here. The reason for the difference is that neither (2.1) nor (5.1) is algebraically "complete" (in the sense of Cartan[26]). That is, for both there exist forms which annihilate the null spaces but do not belong to the ideal. An interesting and important question which is suggested by the WE method is thus to find a complete exterior system whose maximal integral manifolds are the solution manifolds for the original differential equations. If such a system exists, application of the WE method may lead to results of greater generality. There is a second related question: are the pseudopotentials arising from two different differential ideals for the same equation really distinct, or are they necessarily related by dependent variable transformations such as the "inerising" transformation of the type (4.19b)? If they are always so related, there would be no greater generality obtained by changing or extending the ideal. The most general approach, of course, is to return to the method of Clairin,[21,38,48] which works directly with the differential equation, rather than with exterior forms. A comparison of the assumptions involved in these various approaches would be of interest.

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Exact recursion relation for pseudobidimensional arrays of dumbbells

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Exact relationships are developed that describe the occupation statistics for pseudobidimensional arrays of dumbbells. It is found that $E(k,N)$, the number of ways of arranging k indistinguishable dumbbells on a $3\times N$ diagonal array of compartments is exactly described by the recursion relation

$$E(k,N) = 4E(k-1,N-1) + E(k,N-1) - 2E(k-2,N-2).$$

The $3\times N$ diagonal lattice space provides to the central sites of the lattice their full coordination number of nearest-neighboring compartments; therefore the solution of the present system provides a $1\times N$ diagonal (central sites) "window" to watch the behavior of a true bidimensional array of dumbbells. For large values of N, the dumbbell freedom per lattice site on any given site of the central diagonal is found to be 1.8477···, which is only 3% higher than the exact value (1.7916···) found for a "locked" dumbbell on a bidimensional array.

I. INTRODUCTION

Many physical and chemical systems can be represented by the distribution of particles on a lattice space. One interesting problem is to determine statistically the number of possible arrangements of dumbbells (particles that occupy two contiguous lattice sites) on a regular lattice space. We are going to consider a pseudobidimensional lattice space of compartments, and we will allow the dumbbells to occupy two adjacents compartments only. A bidimensional form of this problem is found in the theory of adsorption of diatomic molecules by a metal surface.[1]

Problems dealing with particles that occupy more than one lattice site have always been troublesome; unlike simple particles, there is no reciprocity between particles and vacancies. Therefore, as is generally true for problems of this nature, exact solutions have been found for the one-dimensional case[2–4] but for spaces of higher order dimensionality exact solutions have been obtained only for very special cases—a $2\times N$ rectangular array of compartments,[5] and a bidimensional array completely covered with dumbbells.[6,7]

The purpose of this paper is to study the occupation statistics for dumbbells on a pseudobidimensional lattice space [see Fig. 1(a)]. Unlike the $2\times N$ rectangular lattice space[5] [see Fig. 1(b)] our pseudobidimensional space provides to the central sites of the lattice their full coordination number of nearest neighboring compartments. We are going to determine the occupational degeneracy $E(k,N)$ for dumbbells particles, that is, the number of ways k indistinguishable dumbbells can be arranged on a $3\times N$ diagonal lattice space [see Fig. 1(b)].

II. EXACT RECURSION RELATION

We wish to determine a recursion relation for $E(k,N)$, the number of possible arrangements of k indistinguishable dumbbells on a $3\times N$ diagonal array of compartments. Let us first define the following arrays: (1) An $\epsilon(N)$ array [see Fig. 3(a)] is defined to be an array of compartments arranged in three adjacent diagonals of N compartments each; (2) a $\lambda(N)$ array [see Fig. 3(b)] is one in which the compartments are arranged in three adjacent diagonals of $(N+1)$ compartments for the upper one and N compartments for the other two; (3) a $\gamma(N)$ array [see Fig. 3(c)], as before, an array of compartments arranged in three adjacent diagonals of $(N+2)$, $(N+1)$, and N compartments for the upper, central, and lower diagonals, respectively; (4) a $\delta(N)$ array [see Fig. 3(d)] is an array of three adjacent diagonals of $(N+1)$, $(N+1)$, and N compartments for the upper, central, and lower diagonals, respectively.

Let $E(k,N)$ be the number of ways of arranging k indistinguishable dumbbells on an $\epsilon(N)$ array, and $L(k,N)$, $G(k,N)$, $D(k,N)$ are the number of ways k indistinguishable dumbbells can be arranged on a $\lambda(N)$, $\gamma(N)$, and $\delta(N)$ arrays, respectively.

Theorem I:

$$G(k,N) = D(k,N) + L(k-1,N). \tag{1}$$

Proof: Let $g(k,N)$ be the set of all possible arrangements of k indistinguishable dumbbells on a $\gamma(N)$ array;

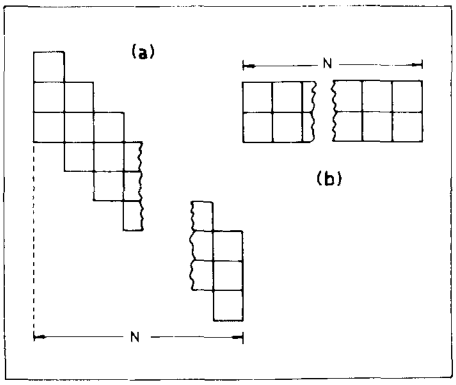

FIG. 1. (a) A $3\times N$ diagonal array; (b) a $2\times N$ rectangular array.

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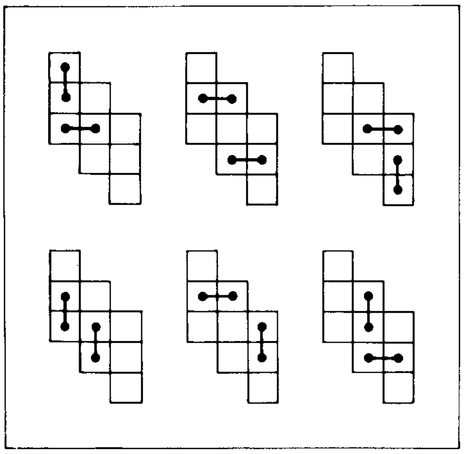

FIG. 2. Six of the 29 possible arrangements of two dumbbells on a 3×3 diagonal array.

$d(k,N)$ is the subset of $g(k,N)$ where the only compartment of the $(N+2)$th column is vacant and $l(k,N)$ is the subset of $g(k,N)$ in which that compartment is occupied. Then, every arrangement in $d(k,N)$ differs from every arrangement in $l(k,N)$ by the condition of occupation of the above mentioned compartment, i.e., $d(k,N)\cap l(k,N)$ is a null set. In addition, every member of $g(k,N)$ can be found either in $d(k,N)$ or $l(k,N)$, i.e., $d(k,N)\cup l(k,N)=g(k,N)$.

Therefore $^*g(k,N)$, the number of members of the set $g(k,N)$, is given by

$$^*g(k,N) = {}^*d(k,N) + {}^*l(k,N) = G(k,N).$$

The compartment of the $(N+2)$th column is unoccupied in the set $d(k,N)$ so that by definition $^*d(k,N)$ is $D(k,N)$. It that compartment is occupied then the adjacent one is also occupied. Hence, all other possible arrangements must involve the remaining $(k-1)$ dumbbells on the remainder of the array, which is a $\lambda(N)$ array. The number of elements in $l(k,N)$ is therefore $L(k-1,N)$, i.e., $^*l(k,N)\equiv L(k-1,N)$.

Therefore, we conclude that

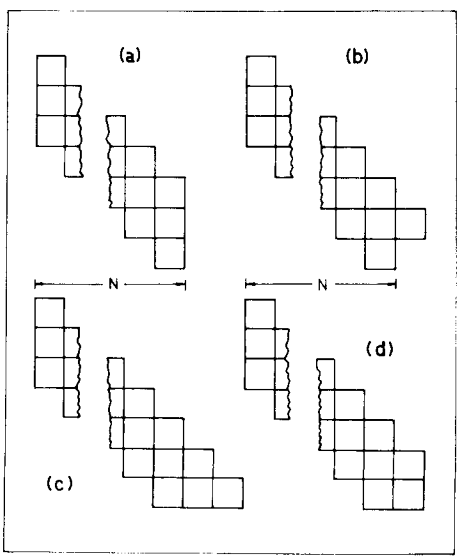

FIG. 3. (a) An $\epsilon(N)$ array, (b) a $\lambda(N)$ array, (c) a $\gamma(N)$ array, and (d) a $\delta(N)$ array.

$$G(k,N) = D(k,N) + L(k-1,N).$$

Theorem II:

$$E(k,N) = D(k,N-1) + L(k-1,N-1) \tag{2}$$

Proof: Let $e(k,N)$ be the set of all possible arrangements of k indistinguishable dumbbells on an $\epsilon(N)$ array; $d(k,N)$ is the subset of $e(k,N)$ where the lower compartment of the Nth column is vacant and $l(k,N)$ is the subset of $e(k,N)$ in which that compartment is occupied. Then, every arrangement in $d(k,N)$ differs from every arrangement in $l(k,N)$ by the condition of occupation of the lower compartment of the Nth column, i.e., $d(k,N)\cap l(k,N)$ is a null set. In addition, every member of $e(k,N)$ can be found either in $d(k,N)$ or $l(k,N)$, i.e., $d(k,N)\cup l(k,N)=e(k,N)$. We conclude that $^*e(k,N)$, the number of members of the set $e(k,N)$, is given by

$$^*e(k,N) = {}^*l(k,N) + {}^*d(k,N).$$

The lower compartment of the Nth column is unoccupied in the set $d(k,N)$, so that by definition $^*d(k,N)$ is $D(k,N-1)$. If that compartment is occupied then the adjacent one is also occupied. Hence, all other possible arrangements must involve the remaining $(k-1)$ dumbbells on the remainder of the array, which is a $\lambda(N-1)$ array. The number of elements in $l(k,N)$ is therefore $L(k-1,N-1)$, i.e., $^*l(k,N)\equiv L(k-1,N-1)$.

Therefore, we conclude that

$$E(k,N) = D(k,N-1) + L(k-1,N-1).$$

Corollary 1:

$$G(k,N-1) = E(k,N) \tag{3}$$

Proof: From Theorem I, substituting N by $N-1$ in Eq. (1), we obtain

$$G(k,N-1) = D(k,N-1) + L(k-1,N-1), \tag{4}$$

and the right-hand side of Eq. (4) is $E(k,N)$ because of Theorem II.

Theorem III:

$$L(k,N) = E(k,N) + L(k-1,N-1). \tag{5}$$

Proof: Let $l(k,N)$ be the set of all possible arrangements of k indistinguishable dumbbells on a $\lambda(N)$ array; $e(k,N)$ is the subset of $l(k,N)$ in which the only compartment of the $(N+1)$th column is vacant and $c(k,N)$ is the subset of $l(k,N)$ in which that compartment is occupied. Then, every arrangement in $e(k,N)$ differs from every arrangement in $c(k,N)$ by the condition of occupation of the only compartment of the $(N+1)$th column, i.e., $e(k,N)\cap c(k,N)$ is a null set. In addition, every member of $l(k,N)$ can be found either in $e(k,N)$ or $c(k,N)$, i.e., $e(k,N)\cup c(k,N)=l(k,N)$. We conclude that $^*l(k,N)$, the number of members of the set $l(k,N)$, is given by

$$^*l(k,N) = {}^*e(k,N) + {}^*c(k,N).$$

Only one compartment of the $(N+1)$th column is vacant in the set $e(k,N)$, so that by definition $^*e(k,N)$ is $E(k,N)$. If that compartment is occupied, then the adjacent one is also occupied. Hence, all other possible arrangements must involve the remaining $(k-1)$ dumbbells on the remainder of the array, which is a $\lambda(N-1)$ array. The number of elements in $c(k,N)$ is therefore $L(k-1,N-1)$, i.e.,

$*c(k,N) = L(k-1,N-1)$.

Therefore,

$$L(k,N) = E(k,N) + L(k-1,N-1).$$

Corollary 2:

$$L(k,N) = \sum_{i=0}^{k} E(k-i,N-i). \tag{6}$$

Proof: We can evaluate $L(k-1,N-1)$ by using Theorem III:

$$L(k-1,N-1) = E(k-1,N-1) + L(k-2,N-2). \tag{7}$$

Substitution of this into the Theorem III yields

$$L(k,N) = E(k,N) + E(k-1,N-1) + L(k-2,N-2).$$

Repeated use of Eq. (7) gives

$$L(k,N) = E(k,N) + E(k-1,N-1) + \ldots + E(1,N-k+1) + L(0,N-k).$$

However, $L(0,N-k) = E(0,N-k)$. Therefore

$$L(k,N) = \sum_{i=0}^{k} E(k-i,N-i).$$

Theorem IV:

$$E(k,N) = L(k,N-1) + L(k-1,N-1) + G(k-1,N-2) + E(k-1,N-1). \tag{8}$$

Proof: Let $e(k,N)$ be the set of all possible arrangements of k dumbbells on an $\epsilon(N)$ array and let $a_1(k,N)$, $a_2(k,N)$, $a_3(k,N)$ and $a_4(k,N)$ be subsets of $e(k,N)$ in which the lower two compartments of the Nth column of the $\epsilon(N)$ array are occupied in a manner shown in Fig. 4. In other words, the $a_i(k,N)$ are defined on the basis of the manner in which those two compartments are occupied. Since every member of a_i(k,N) differs from any and every member of $a_j(k,N)$ $(i\neq j)$ we conclude that $a_i(k,N)\cap a_j(k,N) = \varnothing, i\neq j$. Also, these four configurations are clearly the only possible we can form with the above mentioned compartments; therefore

$$\bigcup_{i=1}^{4} a_i(k,N) = e(k,N).$$

We conclude that

$$*e(k,N) = \sum_{i=1}^{4} *a_i(k,N) \equiv E(k,N). \tag{9}$$

The set $a_1(k,N)$ contains only those arrangements in which those two compartments are vacant. All k dumbbells are then arranged on the remaining $\lambda\,(N-1)$ array; hence $*a_1(k,N) \equiv L(k,N-1)$.

The set $a_2(k,N)$ contains a dumbbell occupying both compartments, and the remaining $(k-1)$ dumbbells are arranged on an array composed of the original array minus the two precluded compartments, i.e., on a $\lambda\,(N-1)$ array. We may then write $*a_2(k,N) \equiv L(k-1,N-1)$.

The set $a_3(k,N)$ has the upper compartment of the above two mentioned occupied and the lower one empty. The remaining end of the dumbbell occupies a compartment of the $(N-1)$th column, the remaining $(k-1)$ dumbbells are arranged on an array composed of the original array minus the three precluded compartments, i.e., on a $\gamma(N-2)$ array. We may then write $*a_3(k,N) \equiv G(k-1,N-2)$.

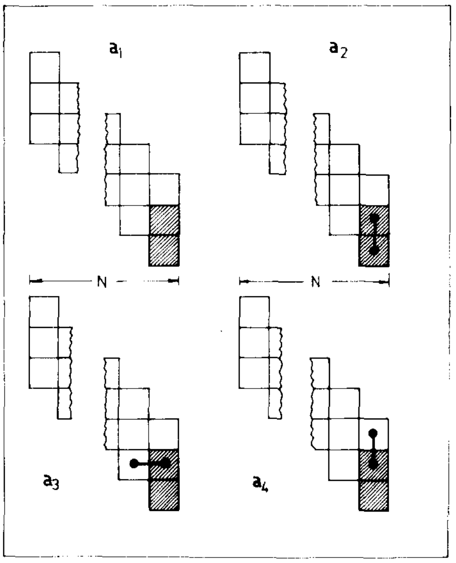

FIG. 4. The four possible states of occupation of the lower compartments of the Nth column.

The set $a_4(k,N)$ has the upper compartment occupied and the lower one empty, the remaining end of the dumbbell occupies another compartment of the Nth column, and the remaining $(k-1)$ dumbbells are arranged on a $\epsilon(N-1)$ array, i.e., $*a_4(k,N) \equiv E(k-1,N-1)$. Therefore, by Eq. (9) we prove Theorem IV.

Corollary 3:

$$E(k,N) = 4E(k-1,N-1) + E(k,N-1) - 2E(k-2,N-2). \tag{10}$$

Proof: By Corollary 1 [Eq. (3)] we evaluate $G(k-1,N-2)$:

$$G(k-1,N-2) = E(k-1,N-1).$$

We may then write Theorem IV as

$$E(k,N) = 2E(k-1,N-1) + L(k,N-1) + L(k-1,N-1).$$

We then use Corollary 2 [Eq. (6)] to evaluate $L(k,N-1)$ and $L(k-1,N-1)$ in Theorem IV, i.e.,

$$E(k,N) = 2E(k-1,N-1) + \sum_{i=0}^{k} E(k-i,N-1-i) + \sum_{i=0}^{k-1} E(k-1-i,N-1-i). \tag{11}$$

If Eq. (11) is used to evaluate $E(k-1,N-1)$, we obtain

$$E(k-1,N-1) = 2E(k-2,N-2) + \sum_{i=0}^{k-1} E(k-1-i,N-2-i) + \sum_{i=0}^{k-2} E(k-2-i,N-2-i).$$

If we form the difference $E(k,N) - E(k-1,N-1)$ and noting that

$$\sum_{i=0}^{k} E(k-i,N-1-i) - \sum_{i=0}^{k-1} E(k-1-i,N-2-i) = E(k,N-1)$$

k \ N	0	1	2	3	4	5	6	7	8	9	10
0	1/2	1	1	1	1	1	1	1	1	1	1
1		2	6	10	14	18	22	26	30	34	38
2			7	29	67	121	191	277	379	497	631
3				24	128	376	832	1560	2624	4088	6016
4					82	536	1906	4992	10850	20792	36386
5						280	2168	9040	27344	67624	145544
6							956	8556	40904	140296	389092
7								3264	33152	178688	685184
8									11144	126640	759584
9										38048	478304
10											129904

FIG. 5. The number of possible arrangements when indistinguishable dumbbells are placed on a $3 \times N$ array for N and k in the range 0–10.

and

$$\sum_{i=0}^{k-1} E(k-1-i, N-1-i) - \sum_{i=0}^{k-2} E(k-2-i, N-2-i) = E(k-1, N-1),$$

we obtain Corollary 3, which is the recursion relation desired.

Corollary 4:

$$E(k,k) = 4E(k-1,k-1) - 2E(k-2,k-2). \quad (12)$$

Proof: Since if $k > N$, no arrangements are possible, i.e., $E(k,N) = 0$, the special case in which the array is $\frac{2}{3}$ filled, or the central diagonal completely filled, has the recursion given by Eq. (12). With the initial conditions $A(0,0) = \frac{1}{2}$ and $A(1,1) = 2$.

Figure 5 shows the number of arrangements of k indistinguishable dumbbells on a $3 \times N$ diagonal array for k and N in the range 0–10, according to Eq. (10) with the boundary conditions $A(k,N) = 0$ (if $k < 0$ and/or $N < 0$; or $k > N$); $A(0,0) = \frac{1}{2}$; $A(1,1) = 2$ and $A(0,1) = 1$.

III. DUMBBELL FREEDOM PER LATTICE SITE

We are going now to compare our results with those obtained on a $2 \times N$ rectangular array[5] and on a bidimensional array.[6,7]

Either the $2 \times N$ rectangular array or the $3 \times N$ diagonal array are very special examples of the physically interesting case of a regular lattice. Nevertheless there is a very important difference between both of them—whereas the sites belonging to the central diagonal in the $3 \times N$ diagonal array have their full coordination number, there is no site with this property on a $2 \times N$ rectangular array. This fact justify the use of the central diagonal of a $3 \times N$ diagonal array as a "window" to watch the behavior of a true bidimensional array of dumbbells.

Let us see how good is this "window" by comparing the dumbbell freedom per lattice site, that is, the number of ways (per lattice site) in which a dumbbell can be placed on the lattice.

The dumbbell freedom per lattice site of a bidimensional array completely covered with dumbbells (which was the only case solved) it was found to be $L_1 = 1.7916...$.[6,7]

In order to perform the comparison we are going to evaluate the dumbbell freedom per lattice site on (i) a completely covered "window" (central diagonal of a $3 \times N$ diagonal array) and (ii) on a completely covered $2 \times N$ rectangular array.

The special case in which the $3 \times N$ diagonal array has its central diagonal completely covered has the recursion relation given by Eq. (12):

$$E(k,k) = 4E(k-1,k-1) - 2E(k-2,k-2).$$

Using the results of Zeitlin,[8] we find the generating function of $E(k,k)$ to be

$$\frac{1}{2 - 8X + 4X^2} = \sum_{k=0}^{\infty} E(k,k) X^k. \quad (13)$$

The generating functions may also be written as

$$\frac{1}{2 - 8X + 4X^2} = \frac{t_1}{1 - T_1 X} + \frac{t_2}{1 - T_2 X}, \quad (14)$$

where the ts are constants and the Ts are the zeros of $2X^2 - 8X + 4$, i.e., $T_1 = 2 + \sqrt{2}$, $T_2 = 2 - \sqrt{2}$.

Therefore, the generating function may be rewritten as

$$\frac{t_1}{1 - T_1 X} + \frac{t_2}{1 - T_2 X} = \sum_{k=0}^{\infty} (t_1 T_1^{\,k} + t_2 T_2^{\,k}) X^k. \quad (15)$$

Since the absolute value of T_2 is less than unity, T_2^k approach zero as $k \to \infty$, therefore

$$\lim_{k \to \infty} E(k,k) = t_1 T_1^k. \quad (16)$$

As $X \to T_1^{-1}$, only the first term on the right-hand side of Eq. (14) is important; therefore

$$\lim_{X \to T_1^{-1}} \left(\frac{1}{2 - 8X + 4X^2} - \frac{t_1}{1 - T_1 X} \right) = 0. \quad (17)$$

By using L'Hospital's rule, we find t_1:

$$t_1 = \frac{T_1^2}{8(T_1 - 1)} = \frac{(2 + \sqrt{2})^2}{8 + 8\sqrt{2}} \simeq 0.603. \quad (18)$$

Therefore we may write

$$\lim_{k \to \infty} E(k,k) = t_1 T_1^k \simeq 0.603(2 + \sqrt{2})^k. \quad (19)$$

The number of occupied sites is $2k$; therefore the $2k$ th root of Eq. (19) is the number of ways (L_2) per lattice site in which a dumbbell can be placed on any given site of the central diagonal.

$$L_2 = \lim_{k \to \infty} [0.603(2 + \sqrt{2})^k]^{1/2k},$$

$$L_2 = \sqrt{2 + \sqrt{2}} \simeq 1.8477....$$

A completely covered $2 \times N$ rectangular array has the following recursion relation (see Ref. 5);

$$A(k,k) = f_k,$$

where f_k is the k th Fibonacci number, proceeding in the same manner as before we find that the dumbbell freedom per lattice site (L_3) of a "locked" dumbbell on a $2 \times N$ rectangular array is 1.2720... .

IV. CONCLUSIONS

The dumbbell freedom per lattice site of a bidimensional array completely covered with dumbbells ($L_1 = 1.7916...$)[6,7] is about 10% lower than 2, which is the number of ways (per lattice site) in which a free dumbbell can be placed on a regular lattice. The corresponding value of any given site of the central diagonal on a $3\times N$ diagonal lattice ($L_2 = 1.8477...$) is only a 3% higher than the exact value. On the other hand, the dumbbell freedom per lattice site on a $2\times N$ rectangular array ($L_3 = 1.2720...$) can never be higher than 1.5, which is the number of ways (per lattice site) in which a free dumbbell can be placed on such an array.

Therefore, we immediately see that the $3\times N$ diagonal lattice can provide a substantial improvement to the understanding of some properties of the physically interesting case of a regular lattice covered with an *arbitrary* number of dumbbells. I hope to comment upon these possibilities in more detail at a later date.

ACKNOWLEDGMENT

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Analytic structure of the Henon–Heiles Hamiltonian in integrable and nonintegrable regimes [a)]

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The solutions of the Henon–Heiles Hamiltonian are investigated in the complex time plane. The use of the "Painlevé property," i.e., the property that the only movable singularities exhibited by the solution are poles, enables successful prediction of the values of the nonlinear coupling parameter for which the system is integrable. Special attention is paid to the structure of the natural boundaries that are found in some of the nonintegrable regimes. These boundaries have a remarkable self-similar structure whose form changes as a function of the nonlinear coupling.

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1. INTRODUCTION

Given a Hamiltonian system there is, as yet, no systematic method for determining whether or not that system is integrable.[1] The usual approach is a combination of numerically investigation and inspired guesswork. However, recent work suggests that there is an intimate connection between the analytic structure of a system and its integrability. This connection was pointed out by Ablowitz *et al.*[2] in the context of partial differential equations (p.d.e.'s). These authors conjectured that if a p.d.e. could be reduced, by an exact similarity transformation, to an ordinary differential equation (o.d.e.) of the Painlevé type, then the associated p.d.e. would be soluble by inverse scattering transform methods, the important characteristics of the Painlevé type o.d.e.'s being that the only movable singularities their solutions can exhibit are simple poles. The importance of this property in the solution of certain dynamical problems was appreciated many years ago in the classical work of Kowalevskaya.[3]

The use of the Painlevé property may also be relevant in determining the integrability of systems of o.d.e.'s. Segur[4] applied this notion to the Lorenz system and was thereby able to identify sets of adjustable parameter values for which there existed one or more integrals of the motion. Recently, two of us[5] made a detailed study of the analytic structure of this system and found that the nonintegrable regimes were characterized by a very rich multisheeted structure.

Here, we report the results of an analysis of the well known Henon–Heiles Hamiltonian. The Painlevé property can also be used in this case to successfully identify those parameter values for which the system is integrable. However, in this paper we are mainly concerned with studying the structure of the *natural boundaries* that appear in the nonintegrable regimes. The existence of such a boundary was recently discussed by Greene and Percival[6] in the context of Hamiltonian maps. These authors have conjectured that natural boundaries may be a generic property of nonintegrable Hamiltonian systems in general. The natural boundaries that we have found for the Henon–Heiles system are remarkable in that they exhibit a self-similar or "fractal"[7] structure that allows one to deduce the form of the singular set. Furthermore, as the system parameters are varied the natural boundary undergoes some remarkable changes with new fractal structures appearing.

2. PAINLEVÉ ANALYSIS AND CANONICAL RESONANCES

We write the Henon–Heiles Hamiltonian in the general form

$$H = \tfrac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) + Dx^2y - C/3)y^3. \qquad (2.1)$$

In the case $D = C = 1$ (2.1) reduces to its standard form.[8] The second order (Newtonian) equations of motion are

$$\ddot{x} = -x - 2Dxy, \qquad (2.2a)$$

$$\ddot{y} = -y - Dx^2 + Cy^2. \qquad (2.2b)$$

We determine the leading order behavior of the solution at a singularity at time $t = t_*$ by making the substitution

$$x = a(t - t_*)^\alpha, \quad y = b(t - t_*)^\beta$$

and equating most singular terms. This leads to the pair of equations

$$\alpha(\alpha - 1)a(t - t_*)^{\alpha - 2} = -2Dab(t - t_*)^{\alpha + \beta}, \qquad (2.3a)$$

$$\beta(\beta - 1)b(t - t_*)^{\beta - 2} = Cb^2(t - t_*)^{2\beta} - Da^2(t - t_*)^{2\alpha}, \qquad (2.3b)$$

with the two sets of solutions

Case 1: $\alpha = -2, \quad a = \pm(3/D)(2 + 1/\lambda)^{1/2},$
$\beta = -2, \quad b = -3/D,$

where for notational convenience we set $\lambda = D/C$, and

Case 2: $\alpha = \tfrac{1}{2} \pm \tfrac{1}{2}(1 - 48\lambda)^{1/2}, \quad a = \text{arbitrary},$
$\beta = -2, \quad b = 6/C.$

Since the most singular behavior supported by the equations of motion is t^{-2}, both branches of the *Case* 2 singularities can only exist for $\lambda > -\tfrac{1}{2}$. For the Painlevé property to hold all leading order behavior must be integers (later we shall show that this constraint may be relaxed), and this places restrictions on the values of λ in *Case* 2. The first few values of λ leading to integer α in this case are $\lambda = -\tfrac{1}{6}, -\tfrac{1}{2}, -1, -\tfrac{5}{3}, \ldots$, etc. Typically, *Case* 2 introduces irrational values of

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λ and for $\lambda > \frac{1}{48}$ the order becomes complex. In the standard case $C = D = 1$ ($\lambda = 1$) we have

$$\alpha = \tfrac{1}{2} \pm (i/2)\sqrt{47}, \quad a = \text{arbitrary}, \tag{2.4a}$$

$$\beta = -2, \quad b = 6. \tag{2.4b}$$

In order to proceed with Painlevé analysis we have to look for the so called *resonances*,[2] i.e., the conditions under which arbitrary parameters may enter into a general power series expansion about $t = t_*$. Since we have two second order equations the solution must be characterized by four constants of integration. One of these is provided by the singularity (hopefully pole) position $t = t_*$. Starting with the *Case* 1 leading orders and following the procedure of Ablowitz *et al.*, we now set

$$x = \pm (3/D)(2 + 1/\lambda)^{1/2} t^{-2} + p t^{-2+r}, \tag{2.5a}$$

$$y = (3/D) t^{-2} + q t^{-2+r}, \tag{2.5b}$$

where p and q are the arbitrary parameters (whose values are fixed by the constants of integration) and for notational convenience we have set $t_* = 0$. These expansions are substituted into the equations of motion (2.2) with only the most singular (dominant) terms included, i.e.,

$$\ddot{x} = -2Dxy, \tag{2.6a}$$

$$\ddot{y} = -Dx^2 + Cy^2. \tag{2.6b}$$

Setting up the ensuing linear equations for p and q one finds, after a little analysis, that these will be arbitrary if

$$\begin{vmatrix} (3-r)(2-r) - 6 & \pm 6(2 + 1/\lambda)^{1/2} \\ \pm 6(2 + 1/\lambda)^{1/2} & (3-r)(2-r) + 6/\lambda \end{vmatrix} = 0. \tag{2.7}$$

Setting

$$\Theta = (3-r)(2-r) \tag{2.8}$$

one finds two possible solutions

$$\Theta = 12 \tag{2.9a}$$

and

$$\Theta = -6(1 + 1/\lambda). \tag{2.9b}$$

These values of Θ determine the values of r (and hence the powers of t) at which the resonances occur.

For $\Theta = 12$ we find

$$r = -1 \text{ or } 6. \tag{2.10}$$

The root $r = -1$ is always present in such analyses and represents the arbitrariness of t_*.[2] This, together with the root $r = 6$, provides us with two of the arbitrary parameters. For $\Theta = -6(1 + 1\lambda)$ we find

$$r = \tfrac{5}{2} \pm \tfrac{1}{2}(1 - 24(1 + 1/\lambda))^{1/2}. \tag{2.11}$$

From this result we see that four-parameter solutions can exist for $\lambda > 0$ or $\lambda < -\frac{1}{2}$. Furthermore the resonances are complex when $\lambda > 0$ or $\lambda < -\frac{24}{23}$ and the imaginary part becomes infinite when $\lambda \to 0^+$.

The resonance analysis may be repeated using the *Case* 2 leading orders. Now the dominant terms in the equations of motion are

$$\ddot{x} = -2Dxy, \tag{2.12a}$$

$$\ddot{y} = Cy^2. \tag{2.12b}$$

The analysis proceeds exactly as before and yields the roots

$$r = -1 \text{ and } 6 \tag{2.13a}$$

and

$$r = 0 \text{ and } r = \mp (1 - 48\lambda)^{1/2}. \tag{2.13b}$$

The upper and lower signs of the last member of (2.13b) are associated with those of the leading order behavior α. In either case the two values of $r + \alpha$ calculated from (2.13b) are equal to the two values of α. The root $r = 0$ corresponds to the arbitrariness of the associated leading order coefficient. Four-parameter solutions can only exist when $\lambda > -\frac{1}{2}$. For $\lambda > \frac{1}{48}$ the leading orders and resonances are complex (the imaginary parts become infinite when $\lambda \to +\infty$). When $-\frac{1}{2} < \lambda \frac{1}{48}$ the negative branch $\alpha_- = \frac{1}{2} - \frac{1}{2}(1 - 48\lambda)^{1/2}$ can define a four-parameter solution; in this range α_- and $r_+ = +(1 - 48\lambda)^{1/2}$ are real. Finally, when $\lambda = 0$ the singularity in the x variable disappears and the equations of motion are integrable.

In order to determine those λ values for which the Painlevé property is satisfied, we require that all leading orders and resonances, for both *Case* 1 and *Case* 2, are integers. The only values of λ for which this can occur are

$$\lambda = -\tfrac{1}{6}, -\tfrac{1}{2}, -1.$$

The value $\lambda = -1$ gives the roots $r = -1, 2, 3, 6$ for the resonances of the *Case* 1 singularities. A detailed analysis of the expansion about the singularity demonstrated that the solution is Painlevé (single valued) and depends on four arbitrary parameters. This implies that the system is integrable and in this case the integrals of motion have been known for some time.[9]

The value $\lambda = -\frac{1}{2}$ is rather peculiar in that the coefficient in the first term of (2.5a) (*Case* 1) vanishes. The resonances for *Case* 1 are $r = -1, 0, 5, 6$. The root $r = 0$ corresponds to the vanishing of the coefficient. What happens is that at $\lambda = -\frac{1}{2}$ the *Case* 1 singularity merges with the positive ($\alpha = 3$) branch of the *Case* 2 singularity. The negative branch ($\alpha = -2$) is undefined at this point. Thus the "leading orders" are $x = at^3$, $y = -3t^{-2}$, where a is arbitrary. There is one resonance at $r = 6$ that introduces one further parameter. Detailed analysis of the expansion about a singularity shows that this is a three-parameter, Painlevé solution and, hence, not the general four-parameter form of the solution.

Finally, we consider the value $\lambda = -\frac{1}{6}$. The resonances of the *Case* 1 singularity are $r = -3, -1, 6, 8$. This implies, and detailed calculation confirms, that the *Case* 1 singularities are associated with a three-parameter, Painlevé form of the solution. On the other hand, for the *Case* 2 singularities ($\alpha = -1, 2$), we find a four-parameter, Painlevé form of solution associated with negative ($\alpha = -1$) branch. By numerical investigation of this case we have found only this four-parameter form of the solution to be present. Motivated by this numerical coincidence, John Greene was able to identify the additional integral of motion for this case, thereby confirming its integrability.[10] The two integrals of motion are the energy

$$E = H = \tfrac{1}{2}(p_x^2 + p_y^2 + Ax^2 + By^2) + x^2y + 2y^3 \tag{2.14}$$

(where for generality we include the variable linear frequencies A and B) and the quantity

$$G = x^4 + 4x^2y^2 - 4\dot{x}(\dot{x}y - \dot{y}x) + 4Ax^2y + (4A - B)(\dot{x}^2 + Ax^2). \quad (2.15)$$

The Painlevé properties of this case, i.e., $\lambda = -\frac{1}{6}$, and the case $\lambda = -1$ have been derived in Ref. 11.

The integrability of the system for $\lambda = -\frac{1}{6}$ raises the interesting question of the significance of the three-parameter solutions. For this particular case this branch of the solution also satisfies the Painlevé property. Numerical investigations, however, could not detect this (three-parameter) solution. It might be possible, then, only to concern oneself with the four-parameter solutions. Thus we have found for the Hamiltonian

$$H = \tfrac{1}{2}(p_x^2 + p_y^2 + Ax^2 + By^2) + Dx^2y - (C/3)y^3, \quad (2.16)$$

with $D/C = -\frac{1}{16}$ and $B = 16A$, that the associated *Case* 2 singularities define, after a trivial change of variables, a four-parameter Painlevé form of the solution. (The details of this calculation are provided in the Appendix). In this case the *Case* 1 singularities also yield a three-parameter branch of the solution which is Painlevé. Although we have not yet found the second integral of motion, the numerical evidence (surfaces-of-section and singularity structure) suggests that this case is indeed integrable. Using this generalized form of Painlevé property there appear to be many parameter values for which the system (2.16) might be integrable.

We now introduce the concept of a *canonical resonance*. In the normal search for resonances one starts with Eqs. (2.5) which utilize the most singular leading order behaviors; in this case $\alpha = \beta = -2$ (*Case* 1). One then proceeds to find the powers of t (that is, $r - 2$) at which the parameters p, q enter the expansion. From (2.11) we see that this power is

$$\tfrac{1}{2} \pm \tfrac{1}{2}(1 - 24(1 + 1/\lambda))^{1/2}. \quad (2.17)$$

By canonical resonance we mean those cases when the power of t at which the resonance occurs is identical to the second possible leading order behavior (*Case* 2). Comparing the square roots in (2.17) and *Case* 2 the only values of λ for which this can occur are

$$\lambda = 1 \text{ and } \lambda = -\tfrac{1}{2}.$$

The case $\lambda = -\frac{1}{2}$ results in a leading order/resonance at $\alpha = 3$ (the root $\alpha = -2$ is discarded). The case $\lambda = 1$ corresponds to the imaginary leading order given in (2.4a). The significance of these canonical resonances would appear to be, on the basis of our numerical results, that the associated analytic structure has a particularly symmetric form. This idea will be illustrated in the next section.

To conclude this section we remark that a study of the detailed structure of a solution about a singularity requires examination of the full series expansions. These are complicated double series. For example, for *Case* 1 leading orders they take the form

$$x(t) = t^{-2} \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} a_{kj} \tau^k t^j + t^{-2} \sum_{k=1}^{\infty} \sum_{j=0}^{\infty} \bar{a}_{kj} \bar{\tau}^k t^j,$$
$$y(t) = t^{-2} \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} b_{kj} \tau^k t^j + t^{-2} \sum_{k=1}^{\infty} \sum_{j=0}^{\infty} \bar{b}_{kj} \bar{\tau}^k t^j, \quad (2.18)$$

where

$$\tau = t^{\alpha}, \quad \alpha = \tfrac{1}{2} + \tfrac{1}{2}(1 - 24(1 + 1/\lambda))^{1/2},$$
$$\bar{\tau} = t^{\bar{\alpha}}, \quad \bar{\alpha} = \tfrac{1}{2} - \tfrac{1}{2}(1 - 24(1 + 1/\lambda))^{1/2},$$

and

$$a_{00} = \pm (3/D)(2 + 1/\lambda)^{1/2}, \quad b_{00} = -3/D.$$

Similar looking series can be written down for the *Case* 2 leading orders. A discussion of the associated recursions relations and the asymptotic ($|t| \ll 1$) properties of the solution near a singularity is beyond the scope of this paper and will be presented elsewhere.[12] However, it is somewhat remarkable and deserves to be noted at this point that (2.18) represents a four-parameter form of the solution when $\lambda > 0$ or $\lambda < -\frac{24}{23}$ (α and $\bar{\alpha}$ complex) or when $-\frac{24}{23} < \lambda < -\frac{1}{2}$ and (α, $\bar{\alpha}$) are not rational.

3. NUMERICAL RESULTS

Many numerical integration techniques proceed with little knowledge of the precise positions and/or orders of the singularities encountered in the complex solution plane. Here we use a Taylor series method that yields detailed information concerning the singularity nearest to the point of integration.[13] The method is automatic in that one only needs to enter a statement of the o.d.e.'s and such control parameters as initial conditions and path of integration. All of the results discussed below were obtained with this method, hereafter referred to as the ATSMCC method.[13] Applied to the Henon-Heiles system ATSMCC was able to locate the positions of the singularities to a high degree of accuracy and evaluate their orders in agreement with our leading order analysis to four figure accuracy or better.

In our preceding note[14] we described the analytic structure of the solutions associated with the canonical case $\lambda = 1$. Here we sample values of λ in the range $+\infty < \lambda - \infty$. In all the results that follow we concentrate on the analytic continuation of $x(t)$. This is the most interesting since there is the possibility of two different leading order behaviors being present. The positions of the singularities are identical for $y(t)$; but here all have the same leading order.

To begin with we will describe the structure of the singularities that occurs when $\lambda = 1$ (canonical resonance). When the solution is expanded at various points along the real-time axis there is found a nonuniform row of seemingly isolated singularities (see Fig. 1). (We specify the initial data so that the motion is bounded for real time and the singularities are a finite distance from the real-time axis.) However, when the path of integration is deformed into the complex-time plane and passes between two of the singularities observed from the real-time axis, there is found a third singularity located at the apex of an (aproximately) isosceles triangle whose base is the line joining the two singularities that are on either side of the path of analytic continuation (see Fig. 1). If this base consists of two order -2 singularities, the singularity at the apex is of order $\frac{1}{2}$. On the other hand, if the base consists of an order -2 and an order $\frac{1}{2}$ (order refers to the real part of the leading order) singularity, there is found an order -2 singularity at the apex. The base angle is found to be approximately 25°.

Furthermore, when one integrates between *any* pair of singularities that are observed to be "neighboring" during the process of analytic continuation, the above construction is repeated. Several levels of structure are implied by this "self-similar" process. One is that the set of singularities consists of a closed, perfect set with no isolated points on the multisheeted Riemann surface. Another is that about any singularity there emanates a double spiral (one clockwise, one anticlockwise) (see Fig. 1). Finally, since the base between the neighboring singularities is contracting geometrically at the successive stages of the analytic continuation process, it is impossible to continue the solution beyond more than a given finite distance in any direction beyond a pair of "base" singularities. That is, assuming one does not retrace the original path, any path of analytic continuation between a pair of singularities (on the same side of the real axis) would appear to be trapped in a geometrically converging web of singularities that creates a natural boundary of the solution. Using the self-similar nature of the above construction, we have estimated the "fractal dimension" of the singular set to be 1.1419 (this calculation is described in Ref. 14).

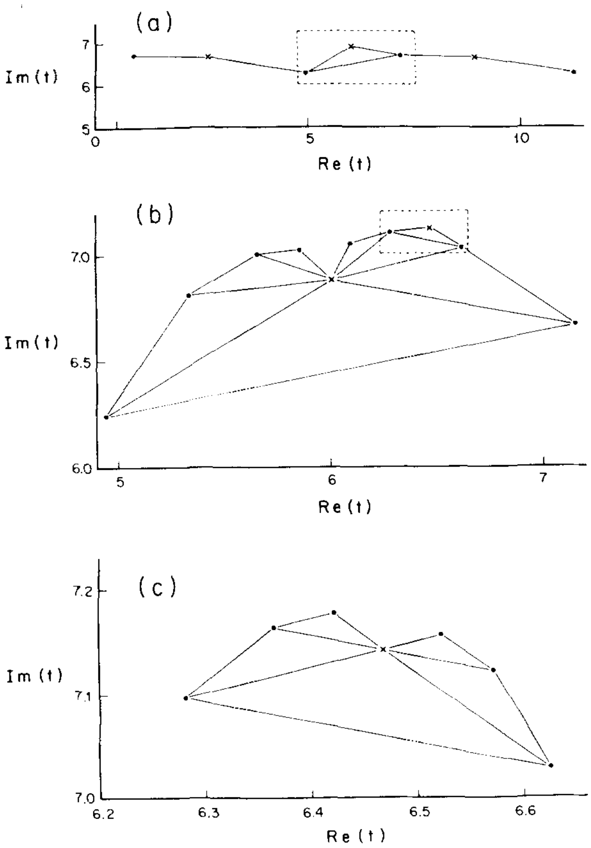


FIG. 1. Analytic continuation of $x(t)$ for $\lambda = 1$. (a) Sequence of singularities found from the real axis and one singularity found at the first stage of analytic continuation. $\cdot$ = singularity of (leading) order -2 and x = singularity of order $\frac{1}{2} \pm (i/2)\sqrt{47}$. (b) Boxed region of (a) in more detail showing double spiral of singularities about apex of "triangle." (c) Boxed region of (b) in more detail showing self-similar nature of the double spiral of singularities. Analytic continuation of $y(t)$ is identical but all singularities now have order-2.

What is particularly striking about the singular structure for $\lambda = 1$ is its highly symmetric form when compared to those found for other values of λ. We believe that this is related to the fact that $\lambda = 1$ is one of the canonical resonances defined in the previous section.[12]

We will now describe the way the singular structure changes at $\lambda \to \infty$. When $\lambda = 1$ there were found two types of triangles: "type 1," whose base consists of two order -2 singularities with an order $\frac{1}{2}$ singularity at the apex, and "type 2," whose base consists of an order -2 and an order $\frac{1}{2}$ singularity with an order -2 apex. As λ increases from 1 the base angles of the type 1 triangles increase (towards 90° when $\lambda \to \infty$) while the base angles of the type 2 triangles decrease (towards 0° as $\lambda \to \infty$). At the same time both type 1 and type 2 triangles cease to be isosceles. The net result is that as $\lambda \to \infty$ the apex of the type 1 triangles recedes infinitely far from the base, which maintains a finite width. The spirals about this apex consist of type 2 triangles, and these collapse onto the sides of the tunnel that is formed by this process. (See Fig. 2.) Along any tunnel the distance between order -2 singularities on the side wall appears to be monotonically decreasing but decreasing sufficiently slowly so that they do not converge in the finite t plane. The overall singular structure when $\lambda \to \infty$ is conjectured to consist of an infinite set of infinitely branched tunnels, constructed entirely of order -2 singularities. The order $\frac{1}{2}$ singularities will be completely inaccessible since they can only be found at the ends of the infinitely deep tunnels. The structure that results is reminiscent of Mandelbrot's generalized Koch curve (Ref. 7, p. 64), which has a fractal dimension of 1.8797.

We have observed that, when $\lambda \to +\infty$ and the imaginary part of the *Case* 2 leading order/resonance becomes infinite, the *Case* 2 singularities recede from the $\lambda = 1$ structure thereby creating a tunneled structure. In a similar way, when λ decreases from 1 to 0 and the imaginary part of the *Case* 1 resonance becomes infinite, the *Case* 1 singularities recede from the original structure creating "tunnels" of *Case* 2 singularities [see Figs. 3 and 4]. The principal differences between the $\lambda \to \infty$ and $\lambda \to 0$ behavior appear to be the integrability of the $\lambda \to 0$ limit and the vanishing of complex *Case* 2 leading order/resonance at $\lambda = \frac{1}{48}$. The vanishing of the complex leading order is associated with the collapse of the type 2 "triangles" into a "sawtooth" structure. [See Fig. 3(e).] At the point of the sawtooth there should appear a *Case* 1 singularity that is a limit point of *Case* 2 singularities that appear on the sides. This sawtooth structure has been found to be repeated between every pair of neighboring *Case* 2 singularities that were studied (sawtooths on sawtooths), thereby implying the existence of a natural boundary (see Fig. 3(f)]. When $\lambda \to 0$ the sawtooth structures are stretched out into a regular lattice by the recession of the *Case* 1 singularities to infinity. (See Fig. 4).

For $-1 \leqslant \lambda \leqslant 0$ there are three values of λ for which the system is integrable:

$$\lambda = 0, \; -\tfrac{1}{6}, \; -1,$$

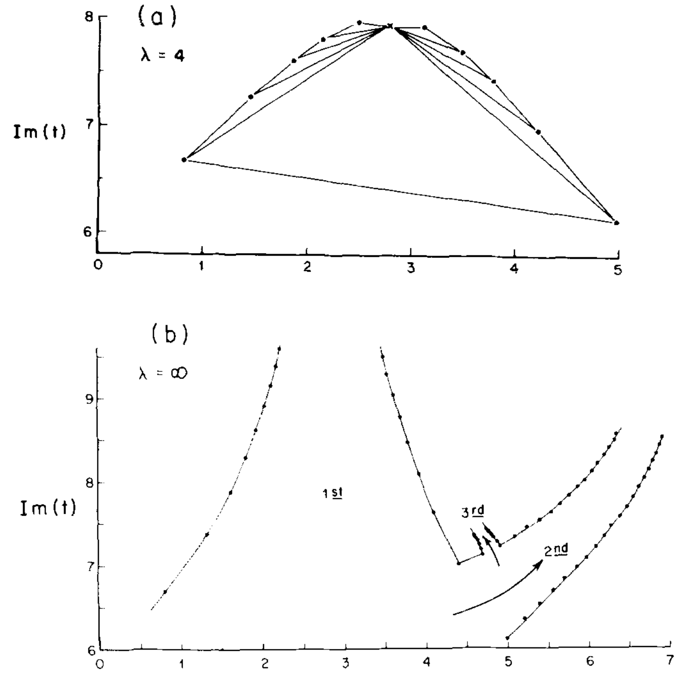
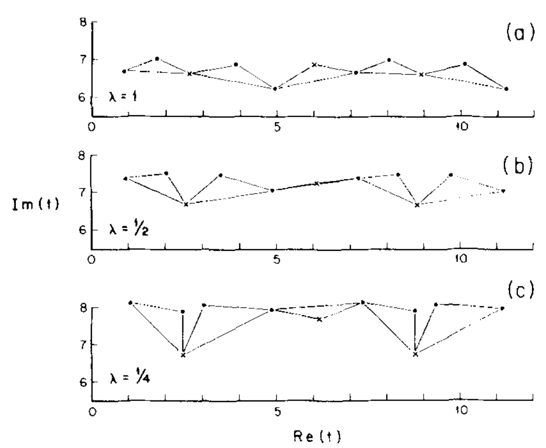


FIG. 2. (a) At $\lambda = 4$ "type 2" triangles collapsing onto sides of "type 1" triangle as the complex singularity (x), now of order $\frac{1}{2} \pm (i/2)\sqrt{191}$, moves deeper into complex plane. (b) At $\lambda = \infty$ the complex singularity has receded to infinity leaving an infinitely deep tunnel with sides made up of singularities of order -2. Tunnels emanate from every pair of adjacent singularities. Here are shown a "primary" (1st) tunnel with associated "secondary" (2nd) and "tertiary" (3rd) tunnels. All lie on the same sheet. Arrows indicate paths of integration.



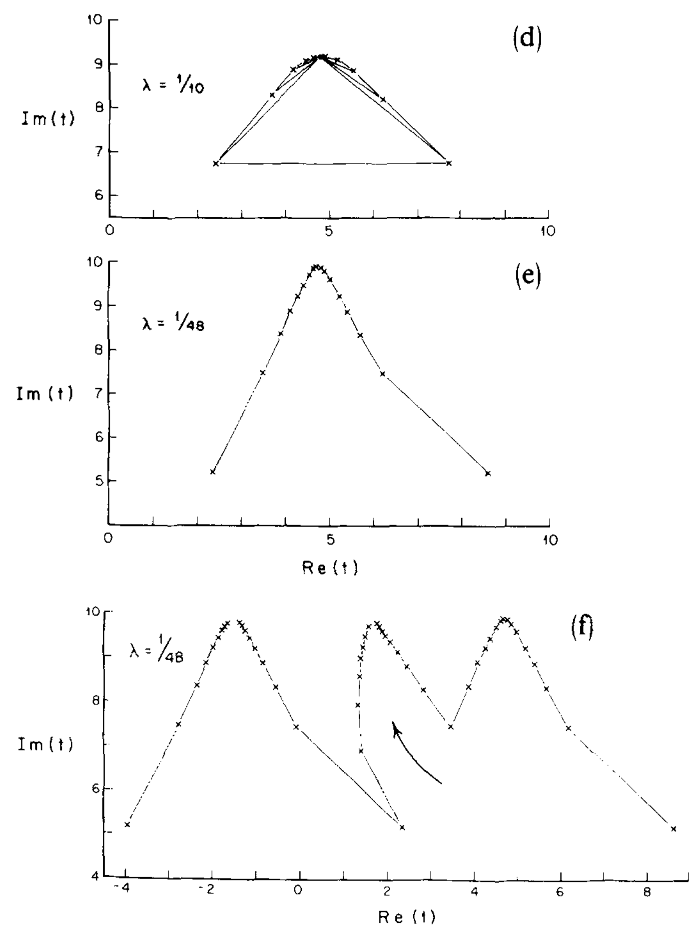


FIG. 3. (a), (b), and (c) positions of *Case* 1 and *Case* 2 singularities gradually changing as λ decreases from 1 to $\frac{1}{4}$. The complex singularities (x) move downwards as the order -2 singularities (·) move away from the real axis. (d) At $\lambda = \frac{1}{10}$ a "principal" triangle with complex (x) base and -2 (·) apex with associated "subsidiary" triangles closing in. (e) At $\lambda = \frac{1}{48}$ the -2 singularities are completely excluded, leaving a sawtooth whose sides are composed entirely of singularities (zeros) of order $\frac{1}{2}$(x). (f) Here are shown a pair of "primary" sawteeth with a "secondary" sawtooth emanating from the side of one of the primaries. Arrow marks path of integration. Note how all the sawteeth pinch off at about the same height, thereby creating a natural boundary.

and one canonical resonance:

$\lambda = -\frac{1}{2}$.

For $-\frac{1}{2} < \lambda \leqslant 0$ the numerical solutions were found to contain solely the negative branch of the *Case* 2 (four-parameter) singularities. For $-1 \leqslant \lambda \leqslant -\frac{1}{2}$ the solution was found to contain *Case* 1 singularities (four-paremeter) only. The significance of this result is that the three-parameter solutions of either case were never found in the numerical solution. It would be of interest to determine what restriction (if any) on the initial data would give rise to these three-parameter forms of the solution. In some instances a three-parameter, Painlevé form of solution (say, for $\lambda = -\frac{1}{2}$) is known, while the general form of the solution is multiple valued. This suggests that by suitably restricting the initial data an "integrable" form of solution might be obtained.

With reference to the above values of λ, the regular lattice of poles found at $\lambda = 0$ [Fig. 4(b)] and $\lambda = -\frac{1}{16}$ distorts into regular clusters of three singularities when $\lambda = -\frac{1}{6}$ (Fig. 5). In this range ($-\frac{1}{6} < \lambda < 0$) we do not find a natural boundary, i.e., it is possible to integrate arbitrarily far into the complex t plane.

In the range $-1 < \lambda < -\frac{1}{6}$ the natural boundary appears to return in a form similar to that found for $0 \leqslant \pm \leqslant \frac{1}{48}$, i.e., a sawtoothlike regularity that is shown in Fig. 6. As λ approaches -1 the sawtooth opens out (the "transition" appears to be around $\lambda = -\frac{3}{4}$) into a regular lattice of poles; lattice points now being pairs of poles (Fig. 7). For this case, as with the cases $\lambda = -\frac{1}{6}$ and $\lambda = 0$, we emphasize that the

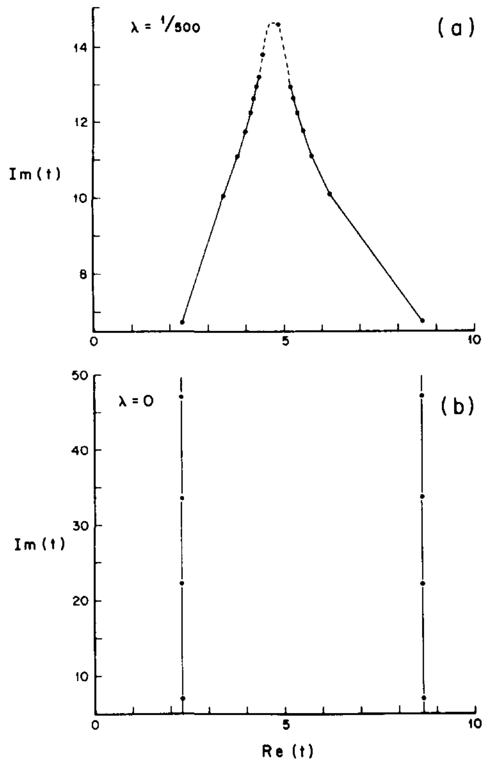


FIG. 4. (a) Elongated sawtooth at $\lambda = \frac{1}{500}$. · = singularity (zero) of order 0.2461···corresponding to the negative branching of the *Case* 2 singularities. (b) Regular lattice of poles at $\lambda = 0$. For $x(t)$ the order is identically zero, for $y(t)$ -2.

soultions are single sheeted.

For λ in the range $-\infty < \lambda < -1$ some quite complicated structures appear but we do not find any natural boundaries. For example, at $\lambda = -6$ we find a "boxing glove" like structure (see Fig. 8) and surprisingly, despite its labyrinthine complexity, it is possible to work one's way through it arbitrarily deep into the complex plane. Finally,

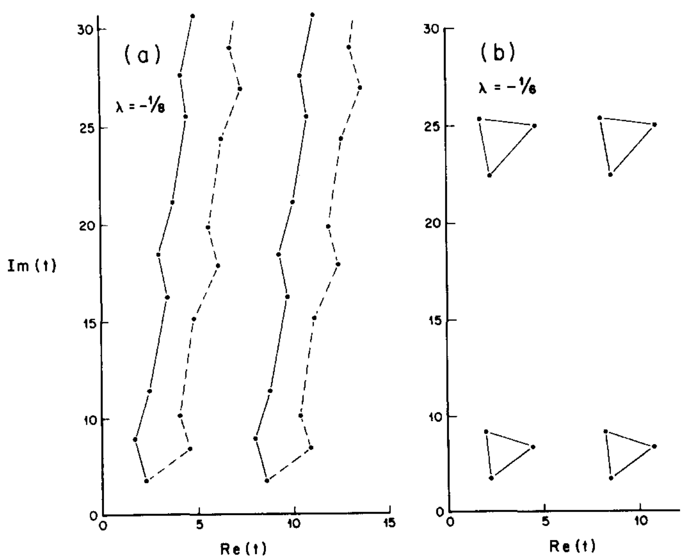


FIG. 5. (a) At $\lambda = -\frac{1}{8}$ rows of singularities [order $(1-\sqrt{7})/2$]. Dotted line indicates positions of singularities as integrator approaches from right and full line for approach from left. (b) At $\lambda = -\frac{1}{6}$ regular lattice of triads of poles, all of order -1.

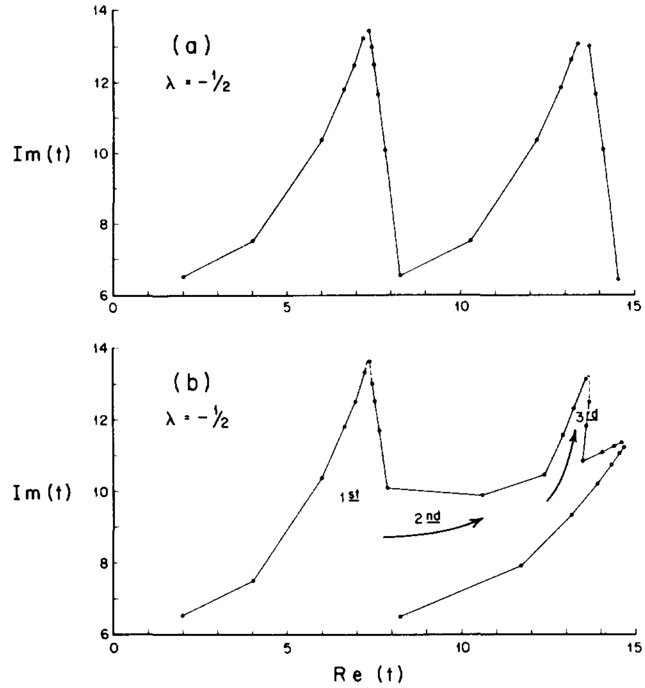


FIG. 6. (a) At $\lambda = -\frac{1}{2}$ sawteeth of singularities now of order -2. The pattern repeats with remarkable regularity. (b) Secondary and tertiary sawteeth emanating from side of the left-hand sawtooth in (a). The system of these connecting tunnels lies on same sheet. Arrows mark paths of integration.

at $\lambda = -\infty$ we find an infinitely deep tunnel-like structure similar to that found at $\lambda = +\infty$.

Our results suggest that the overall changes in the analytic structure can be divided into four main ranges:

(i) $0 < \lambda \leqslant +\infty$ natural boundary present,
(ii) $-\frac{1}{6} \leqslant \lambda \leqslant 0$ *no* natural boundary present,
(iii) $-\frac{3}{4} < \lambda < -\frac{1}{6}$ natural boundary present,
(iv) $-\infty < \lambda < -\frac{3}{4}$ *no* natural boundary present,

although ranges (iii) and (iv) have not been investigated in any detail.

To conclude we note the results of a number of tests (by

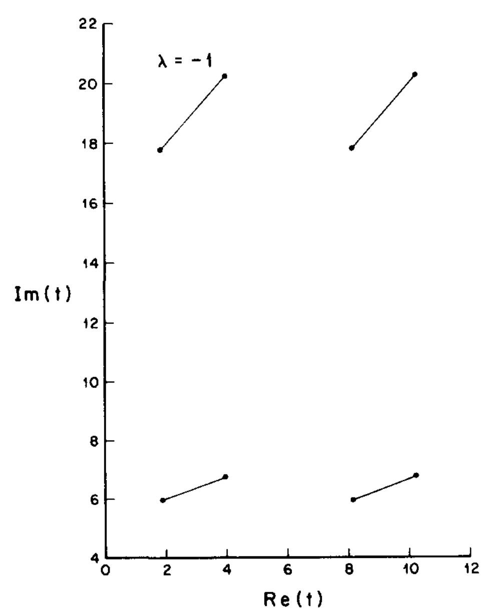


FIG. 7. At $\lambda = -1$ regular lattice of doublets of poles of order -2.

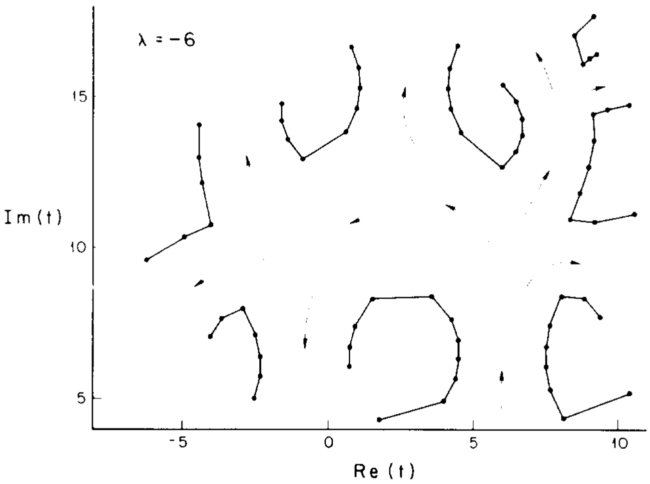


FIG. 8. $\lambda = -6$ showing complicated "boxing glove" structure of singularities. Arrows indicate paths of integration.

no means complete) that were made of the effect of changes in initial conditions and energy on the various structures described above. Changes in the former (at a given energy) tended to twist or tilt the structures slightly, and increases in the latter tended, overall, to bring them slightly closer to the real axis. In general, however, the basic geometry of the structures is unchanged.

ACKNOWLEDGMENTS

We would like to thank Professor J. M. Greene for useful discussions and for providing us with Eq. (2.15).

APPENDIX: GENERALIZED PAINLEVÉ PROPERTY

We consider Henon–Heiles systems of the form

$$H = \tfrac{1}{2}(p_x^2 + p_y^2 + Ax^2 + By^2) + Dx^2y - (C/3)y^3, \quad \text{(A1)}$$

with the equations of motion

$$\ddot{x} = -Ax - 2Dxy,$$
$$\ddot{y} = -By - Dx^2 + Cy^2. \quad \text{(A2)}$$

In the parameter range $-\frac{1}{2} < \lambda < 0 (\lambda = D/C)$ the *Case* 2 singularities, with leading order behavior

$$x = at^{\alpha}, \quad \alpha = \tfrac{1}{2} - \tfrac{1}{2}(1 - 48\lambda)^{1/2},$$
$$y = bt^{-2},$$

have resonances at

$$r = -1, 0, (1 - 48\lambda)^{1/2}, 6,$$

which defines a four-parameter form of the solution. On the other hand, the *Case* 1 singularities can define, at most, a three-parameter solution.

We find that for

$$\lambda = -\tfrac{1}{16}$$

the *Case* 2 leading order

$$\alpha = -\tfrac{1}{2}$$

and resonances

$$r = -1, 0, 2, 6.$$

By requiring that

$$B = 16A$$

the expansions at the *Case* 2 singularities are found to be

$$x(t) = t^{-1/2} \sum_{j=0}^{\infty} a_j t^j,$$
$$y(t) = t^{-2} \sum_{j=0}^{\infty} b_j t^j,$$

where

j	a_j	b_j
0	μ	$-\frac{3}{8}$
1	0	0
2	θ	$-A/2$
3	$-\mu^3/18$	$\mu^2/12$
4	$(\mu/5)A^2$	$-\frac{4}{5}A^2$
5	$-\mu^2\theta/18$	$\mu\theta/3$
6	$\frac{1}{24}(\mu^5/108 - 2\mu\psi)$	ψ

and μ, θ, ψ are arbitrary. In terms of the variable $\tau = t^{1/2}$ the above expansion are Painlevé. For the *Case* 1 singularities we find that

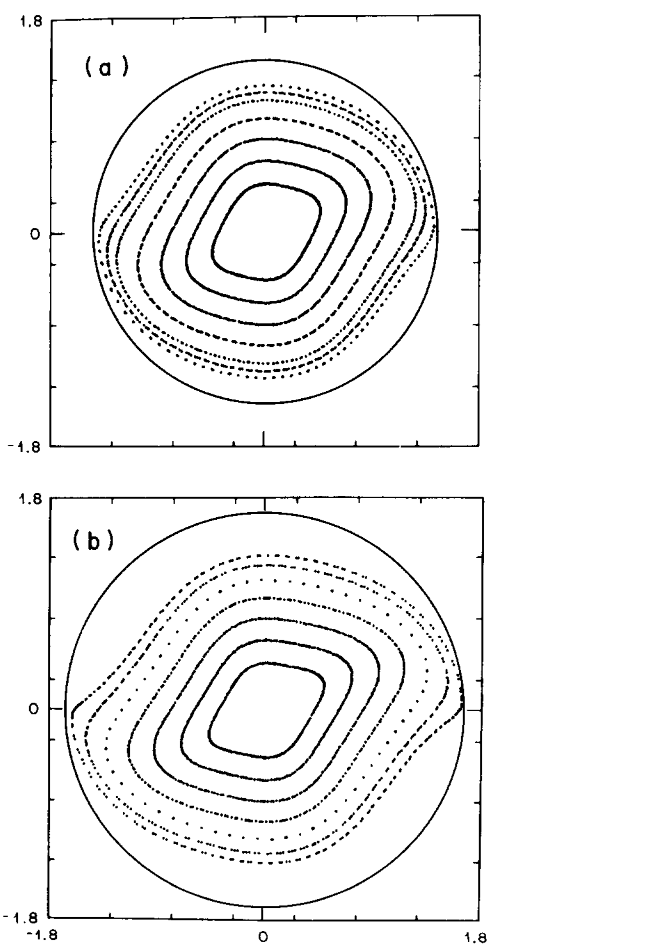


FIG. 9. Surface-of-section of Henon–Heiles system with $D = 1$, $C = -16$, $A = 1$, $B = 16$ at (a) $E = 1$ and (b) $E = \frac{4}{3}$ (dissociation). Outermost circle denotes phase space boundary. In the outermost regions we found smooth, densely packed, banana shaped curves. There were no discernable regions of chaotic motion.

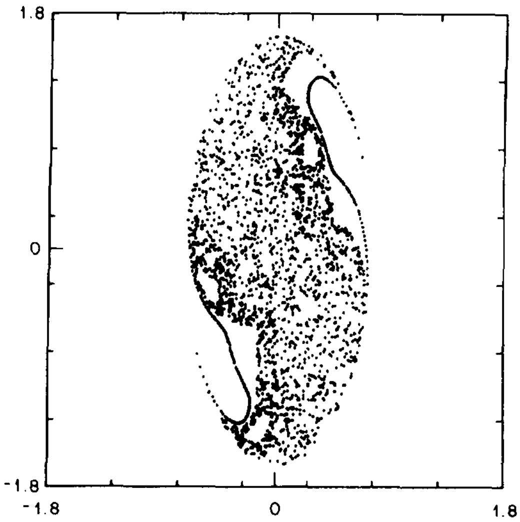


FIG. 10. Surface-of-section of Henon–Heiles system with $D = 5$, $C = -16, A = 5, B = 16$ at $E = \frac{4}{3}$ (dissociation). By contrast with Fig. 9(b) there are large regions of chaotic motion.

$$x \simeq \pm 3i(14)^{1/2} t^{-2},$$
$$y \simeq -3t^{-2}$$

with resonances

$$r = -1,\ 6,\ \tfrac{5}{2} \pm \tfrac{1}{2}\sqrt{361}.$$

Suprisingly, this branch is also of the Painlevé form (albeit three-parameter). We have studied the surfaces-of-section (see Fig. 9) and these show only smooth invariant curves, right up to the dissociation threshold ($E = \frac{4}{3}$). The singularity structure of the solutions is always that of a regular lattice. These results are strongly indicative of an integrable system. (We add that surfaces-of-section for other λ values around $\lambda = -\frac{1}{16}$ were also very smooth.)

These results for $\lambda = -\frac{1}{16}$ clearly suggest that there may be many other integrable cases (for $\lambda < 0$). Thus, in the range $-\frac{1}{2} < \lambda < 0$, any λ value for which

$$(1 - 48\lambda)^{1/2} = n/m, \tag{A3}$$

where n and m are (relatively prime) integers, may yield a four-parameter Painlevé solution in the variable $\tau = t^{1/2m}$. However, each case must be checked for logarithmic terms. Thus, for example, $\lambda = \frac{5}{16}$, which satisfies (A3), is found not to be Painlevé. A surface-of-section at the dissociation threshold (also $E = \frac{4}{3}$ when $A = 5$, $B = 16$) shows widespread chaos for this case (see Fig. 10).

In the range $-\frac{24}{23} < \lambda < -\frac{1}{2}$ for which only the *Case* 1 singularities yield (real) four-parameter solutions, there is also the possibility of Painlevé solutions for those λ values satisfying

$$(1 - 24(1 + 1/\lambda))^{1/2} = n/m. \tag{A4}$$

One possible candidate is $\lambda = -\frac{3}{4}$. However, direct calculation reveals that this is also not Painlevé. A systematic study of all the cases satisfying (A3) and (A4) is currently in progress.

Note added in proof: We have recently learned that L. S. Hall (Lawrence Livermore Laboratory, Preprint UCID-18980, 1982) has found, by another method, the second integral of motion for the case $\lambda = -\frac{1}{16}$.

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Classical mechanics of nonspherical bodies. I. Binary collisions in two dimensions

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In order to discuss the statistical mechanics and to prove an H-theorem for two-dimensional, nonspherical bodies, which possess only a symmetry axis, the mechanics of collisions of such bodies are investigated in detail, starting from the collision formulae of D. Bernoulli and Euler.

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I. INTRODUCTION

A. Introductory remark

The present work is concerned with two-dimensional rigid bodies. Rigid means that all inner (elastic) degrees of freedom are neglected; thus its motion can still be formulated in terms of ordinary differential equations. In two dimensions, the essential new feature of the collision problem for asymmetric bodies, namely transfer of angular momentum, is present, but without some of the technical complications that occur in three dimensions (tensor instead of a scalar moment of inertia, pseudovector instead of a pseudoscalar angular velocity). Therefore, all theorems are formulated here for two dimensions; a three-dimensional treatment will follow.

B. Outline of the paper

In a previous publication,[1] one of the authors (D.S.) recalled a classical equation describing binary collisions of two-dimensional rigid bodies due to Daniel Bernoulli and Euler (1737); here we present a modern derivation of these equations. Apart from their interest and their use as classical models for nonspherical molecules, these collision equations can be used for the statistical mechanics of large systems of such bodies.[2] In three dimensions, such problems were largely discussed in the classical treatises of Boltzmann[3] and Tolman[4]; however, the derivation of the collision equations is generally shunted.

For this reason, and because it has not been published yet for two-dimensional bodies, we present in Secs. II–IV a derivation of the collision equations. In Sec. II, the main properties of two-dimensional rigid bodies are presented. Section III complements it by expliciting the geometrical notions needed to describe a binary collision: On the one hand, the full description is given by the constellation of the collision; on the other hand, the relevant dynamical parameters are the impact parameters. The dynamics of a binary collision will not be discussed in the present paper, but the kinematics are presented in Sec. IV, in which the collision equations are derived (from hypotheses which make the notion "rigid" explicit); a compact description is given in terms of the Eulerian collision matrix, whose properties will be discussed.

One of the crucial problems of kinetic theory as well as of collision dynamics is, of course, reversibility. In the present framework, one must ask whether any given collision (which causes a change of state of two bodies) may be compensated by some other collision. Lorentz[5] noticed that compensating collisions do not always exist for bodies of arbitrary shapes. Though Lorentz's argument closely parallels Euler's methods, it seems that he did not carry it through. However, Tolman shows that, under some symmetry assumptions on the shapes, compensating collisions do exist in three dimensions.

In the framework of quantum mechanics, a similar problem was treated by Stückelberg[6] and Heitler,[7] who related the problem of reversibility (and of compensating collisions) to the unitarity of the scattering matrix.

In the present work, a general discussion of the problem of compensating collisions is given in terms of the impact parameters (instead of the constellations themselves) in Sec. V. In Sec. VI, a sufficient condition for the existence of compensating collisions is derived for bodies with a reflection symmetry (i.e., an axis symmetry).

The paper ends with some remarks about questions which remain open.

C. Remarks on the notation: scalars, vectors, and pseudoscalars

A scalar is denoted by an italic letter: v
A vector is denoted by a boldface roman letter: $\mathbf{v}$
The modulus of vector $\mathbf{v}$ is $v \equiv |\mathbf{v}| = (\mathbf{v}\cdot\mathbf{v})^{1/2}$
The scalar product of two vectors $\mathbf{v}$ and $\mathbf{b}$ is: $\mathbf{v}\cdot\mathbf{b}$
A pseudoscalar is denoted by a script letter: $\mathscr{I}$
$\hat{e}_1, \hat{e}_2$ are two orthogonal unit vectors (in clockwise order)
$\hat{\epsilon}$ is the pseudoscalar unity
$\times$ denotes the external product:

$$\hat{\epsilon} = \hat{e}_1 \times \hat{e}_2 = -\hat{e}_2 \times \hat{e}_1,$$
$$\hat{e}_1 = \hat{e}_2 \times \hat{\epsilon} = -\hat{\epsilon} \times \hat{e}_2,$$
$$\hat{e}_2 = \hat{\epsilon} \times \hat{e}_1 = -\hat{e}_1 \times \hat{\epsilon}.$$

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This external product defines a clockwise orientation of the plane.

II. THE ISOLATED TWO-DIMENSIONAL RIGID BODY

A. Geometry

A two-dimensional rigid body is, with respect to collisions, completely specified by:

—its shape, i.e., its boundary, which may be given as a closed curve in the plane,

—the location of its center of mass (c.m.), which is arbitrary within the boundary,

—its mass m,

—its moment of inertia around the c.m., θ, or alternatively its radius of gyration $g \equiv (\theta/m)^{1/2}$.

Whereas the shape is a purely geometric quantity, the location of the c.m. depends on the mass distribution inside the body. This mass distribution, however, enters into the formula that describes the collision process only through m and θ. It is convenient to describe the boundary of the body with the help of polar, *body-fixed* coordinates (r,ψ), the origin of which is located at the c.m. The reference direction $(\psi = 0)$ will be fixed later. In this section it remains arbitrary.

Let the boundary be given by a relation $r = r(\psi)$. In what follows we assume that

(1) the body is convex;

(2) the boundary is sufficiently smooth, i.e., twice continuously differentiable.

The first condition implies that the function $r = r(\psi)$ is a univalued, positive function. Because of the second condition, the curvature exists and is a continuous function of ψ:

$$\kappa = \kappa(\psi) = \frac{-rr'' + 2r'^2 + r^2}{(r'^2 + r^2)^{3/2}}, \tag{2.1}$$

where the prime denotes derivation with respect to ψ. The body is convex if

$$\kappa \geqslant 0 \tag{2.2a}$$

i.e.,

$$rr'' - r'^2 \leqslant r^2 + r'^2. \tag{2.2b}$$

If the inequality holds strictly, we shall call the body strictly convex; we shall restrict ourselves to this special case.

A boundary point Q then is parametrized by the angle ψ or, what amounts to the same, by the length of the segment of the boundary, such that

$$l\,[Q(0)] = 0, \tag{2.3a}$$

$$l\,[Q(\psi_0)] = \int_0^{\psi_0} l\,'(\psi)\,d\psi, \tag{2.3b}$$

with

$$l\,'(\psi) \equiv (r^2 + r'^2)^{1/2}. \tag{2.4}$$

The total length is

$$L = l\,[Q(2\pi)]. \tag{2.5}$$

In the following, we shall simply write $l(\psi)$ instead of $l\,[Q(\psi)]$ and all equalities referring to l will be understood "modulo L" (just like all equalities referring to ψ are understood modulo 2π).

B. Impact parameters

If the body is hit at a point $Q(\psi)$, the impact vector $\mathbf{b}$ is given by

$$\mathbf{b} = \beta\hat{u}, \tag{2.6}$$

and the lever scalar β by

$$\beta(\psi) = rr'/l\,', \tag{2.7}$$

where $\hat{u}$ is the unit vector directed along the tangent to the boundary at $Q(\psi)$ (followed anticlockwise). If one defines an inward normal unit vector $\hat{n}$ at point Q, one finds

$$\begin{aligned} \hat{u} &= \hat{n}\times\hat{\epsilon}, \\ \hat{\epsilon} &= \hat{u}\times\hat{n}, \\ \hat{n} &= \hat{\epsilon}\times\hat{u}. \end{aligned} \tag{2.8}$$

Obviously, for a convex body, $\hat{u}$ and $\hat{n}$ are uniquely determined by Q (or ψ or l), and conversely (see Fig. 1). Similarly, b and β are uniquely determined by Q (or ψ or l), *but the converse does not hold.*

Definition 1: Let Q_1 be a boundary point; consider the set B_1 of all boundary points Q_i such that

$$b_i = b_1.$$

Hence

$$\beta_i = \sigma_i\,\beta_1 \tag{2.9}$$

with

$$\sigma_i = \pm 1$$

and we define two subsets of B_1

if $\sigma_i = +1$: Q_i is said to be equivalent to Q_1,

if $\sigma_i = -1$: Q_i is said to be antiequivalent to Q_1.

Obviously, in both cases,

$$\mathbf{b}_1\times\hat{n}_1 = \sigma_i\mathbf{b}_i\times\hat{n}_i. \tag{2.10}$$

Definition 2: A point Q is called indifferent if $b(Q) = 0$. Obviously, if Q_1 and Q_2 are equivalent *and* antiequivalent, they are indifferent.

C. State of a body

The kinematical state of a rigid body is determined by four parameters:

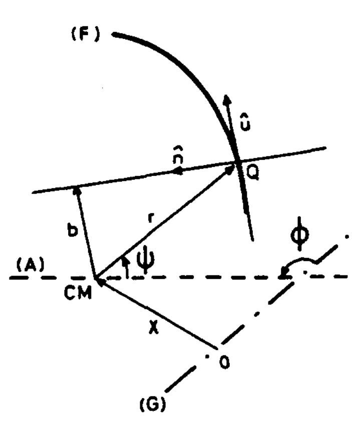

FIG. 1. Description of a rigid body: (G) reference axis in the plane ($\phi = 0$), (A) body-fixed axis ($\psi = 0$), (F) boundary of the body.

—the location of the c.m., given by a vector $\mathbf{x}$ in the plane;

—the direction of the bodyfixed reference axis ($\psi = 0$); it will be given by the angle ϕ between the body-fixed axis and the space-fixed x axis;

—the velocity of its c.m.: $\mathbf{v}\equiv\dot{\mathbf{x}}$

—its angular velocity around the c.m.: $\omega\equiv\dot{\phi}$

The position $\mathbf{x}$ and the velocity $\mathbf{v}$ are vectors. The direction ϕ (the difference of two direction parameters) and the angular velocity ω are pseudoscalars. Any point on the boundary has a location in the plane given by

$$\mathbf{Q}(\psi) = \mathbf{x} + \mathbf{r}(\psi), \tag{2.11}$$

where

$$|\mathbf{r}| = r(\psi), \quad \arg \mathbf{r} = \psi + \phi.$$

We shall denote the state of a body by $\mathbf{S}$:

$$\mathbf{S}\equiv(\mathbf{x},\phi,\mathbf{v},\omega).$$

Obviously, the state is a function of time: $\mathbf{S} = \mathbf{S}(t)$.

The canonical momenta are

$$\text{the linear momentum} \quad \mathbf{p}\equiv m\mathbf{v}, \tag{2.12a}$$

$$\text{the intrinsic momentum} \quad s\equiv\theta\omega, \tag{2.12b}$$

$$\text{the angular momentum} \quad \ell = s + \mathbf{x}\times\mathbf{p}. \tag{2.12c}$$

For a body in a force field $\mathbf{F}$ and a torque field $\mathscr{M}$:

$$d_t \mathbf{p} = \mathbf{F}, \tag{2.13a}$$

$$d_t\, s = \mathscr{M}. \tag{2.13b}$$

The following notations will be used:

$\mathsf{x} = (\mathbf{x},\phi)$ "complete location,"

$\mathsf{v} = (\mathbf{v},\omega)$ "complete velocity,"

$\mathsf{p} = (\mathbf{p}, s)$ "complete momentum,"

$\mathsf{y} = (\phi,\mathbf{v},\omega)$ "abstract location."

Finally, we introduce the kinetic energy

$$E\equiv\frac{1}{2m}p^2 + \frac{1}{2\theta}s^2 = \tfrac{1}{2}mv^2 + \tfrac{1}{2}\theta\omega^2. \tag{2.14}$$

III. GEOMETRY FOR A BINARY COLLISION

A. Description of a collision

Consider two rigid bodies 1 and 2 in states $\mathbf{S}_1^-$ and $\mathbf{S}_2^-$ at time $t < t_0$; the two bodies need not be identical. Moreover, we neglect the influence of any "external fields" of force and moment in some interval including the time of the collision t_0: In this interval, the bodies are free, except for collisions; we always refer to times in this interval. We shall write down a collision in the obvious notation

$$\mathbf{S}_1^- + \mathbf{S}_2^- \underset{t=t_0}{\rightarrow} \mathbf{S}_1^+ + \mathbf{S}_2^+. \tag{3.1a}$$

If a collision occurs, $\mathbf{x}$ and ϕ vary continuously, while $\mathbf{v}$ and ω jump. These jumps can be described by vector-valued step functions. The complete locations of both bodies are therefore well defined at the time of the collision. If we call them X_i^0 ($i = 1,2$), their evolution X_i before and after the collision may be written as:

before the collision ($t < t_0$),

$$\mathsf{X}_i^- = \mathsf{X}_i^0 + \mathsf{V}_i^-(t - t_0); \tag{3.1b}$$

after the collision ($t > t_0$),

$$\mathsf{X}_i^+ = \mathsf{X}_i^0 + \mathsf{V}_i^+(t - t_0). \tag{3.1c}$$

Equations (3.1) express the hypothesis of instantaneous collisions. Therefore, a proper description of the bodies at instant t_0, the only one at which they interact, is crucial.

B. Constellations

The relative position of two colliding rigid bodies (1 and 2) is given by standard variables $(\mathbf{x}_1,\phi_1)$ and $(\mathbf{x}_2,\phi_2)$. At time t_0 the bodies have one single common boundary point Q, where the impact occurs; we distinguish between Q_1 (the boundary point on body 1), Q_2 (on body 2), and Q (the point of the plane which coincide with Q_1 and Q_2 at time t_0). Knowing Q_i is equivalent to knowing the angle ψ_i (see Sec. II B) provided also ϕ_i is known; if one knows the shape of the bodies, it is easy to derive from Q, ψ_i, and ϕ_i the location $\mathbf{x}_i$ of the c.m.

Moreover, since the boundaries are continuously differentiable, they have a common tangent at the impact point:

$$\hat{n}_1 // \hat{n}_2.$$

As the bodies are on opposite sides of the tangent,

$$\hat{n}_1 + \hat{n}_2 = 0; \tag{3.2a}$$

hence

$$\hat{u}_1 + \hat{u}_2 = 0. \tag{3.2b}$$

Since the normal vector $\hat{n}_i$ and the direction parameter ψ_i fix the boundary point Q_i completely, the geometry of the collision can be completely reconstructed from the following data:

—the location of the impact in the plane: Q

—the relative positions of the bodies, i.e., the constellation (ϕ_1,ϕ_2,Q_1).

Since the constellation is defined at the time of the impact, it is called (after Boltzmann,[3] Sec. 79) the critical constellation. Because of its role for the description of collision (3.1), we shall indicate it in the collision formula through the symbol Q_1 (or l_1):

$$\mathbf{S}_1^- + \mathbf{S}_2^- \underset{t=t_0}{\overset{(Q_1)}{\rightarrow}} \mathbf{S}_1^+ + \mathbf{S}_2^+. \tag{3.3}$$

C. Impact parameters

From the critical constellation (ϕ_1,ϕ_2, l_1), it is easy to derive the impact parameters for each body; they are the vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. However, since the bodies are tangent to each other, there are only three independent impact parameters:

—two scalars β_1 and β_2,

—one unit vector $\hat{n}_1$ (or $\hat{n}_2$, e.g.).

Four possible relations between constellations are useful for what follows.

Definition 3: Two constellations $(\phi_1^k,\phi_2^k, l_1^k)$ $(k = A,B)$ are called:

—congruent if $\beta_i^A = \beta_i^B$ $(i = 1,2)$,

—anticongruent if $\beta_i^A = -\beta_i^B$ $(i = 1,2)$,

—equivalent if $\beta_i^A = \beta_i^B$ and $\hat{n}_i^A = \hat{n}_i^B$ $(i = 1,2)$,

—antiequivalent if $\beta_i^A = -\beta_i^B$ and $\hat{n}_i^A = -\hat{n}_i^B$ $(i = 1,2)$.

This classification parallels Tolman's classification of constellations; however, Boltzmann and Tolman take as fundamental parameters the relative positions of the bodies, whereas we relate the classification to the more relevant impact parameters. Therefore, we shall not retain their vocabulary.

As for boundary points, we notice that the existence of constellations anticongruent to a given one is not granted in general (that is, for bodies of arbitrary shape). In fact, it does *not* exist in general. In Sec. VI we shall derive a sufficient condition with respect to the shapes of two bodies which guarantees the existence of an anticongruent constellation whatever the direct constellation.

Proposition 1: Given a constellation (ϕ_1,ϕ_2, l_1) and an arbitrary angle ϕ_0, the constellation $(\phi_1 + \phi_0,\phi_2 + \phi_0, l_1)$ is congruent to (ϕ_1,ϕ_2, l_1).

Proof: Obvious; this is nothing but rotational invariance!

Corollary: One may associate an infinite one-parameter family of mutually congruent constellations $(\phi_1^{=},\phi_2^{=}, l_1^{=})$ with any given constellation (ϕ_1,ϕ_2, l_1); this family will be indexed by one angle parameter.

Furthermore

$$dl_1^{=} = dl_1, \quad d\phi_1^{=} = d\phi_1, \quad d\phi_2^{=} = d\phi_2. \tag{3.4}$$

IV. THE COLLISION EQUATIONS

The collision equations, relating the incoming and outgoing states of two bodies can be derived in various ways. The problem of their derivation may be stated as follows:

(1) The incoming (as well as the outgoing) state is given by six dynamical variables: the two vectors $(\mathbf{p}_1,\mathbf{p}_2)$ and the two pseudoscalars $(\not{s}_1,\not{s}_2)$.

(2) There are four conservation laws, valid for free system:

—one vector $(\mathbf{p}_1 + \mathbf{p}_2)$,

—one pseudoscalar $(\not{s}_1 + \not{s}_2)$,

—one scalar $(E_1 + E_2)$.

Therefore, one must find two more relations for connecting incoming and outgoing states in order to have a complete description of the collision. But it is known that the outgoing momenta $(\mathbf{p}_1,\mathbf{p}_2)$ depend also on the constellation, which is characterized by the impact parameters; thus collision formulae must provide relations between incoming and outgoing momenta, in which the impact parameters enter explicitly.

Such relations always rest on the hypotheses through which the physical (mechanical) notion of "rigid body" is formulated. Several derivations have been proposed (see Ref. 1b for a discussion); the following one seems the shortest since all (including the constitutive) hypotheses are formulated with the help of the momenta.

A. The collision equations for momenta

Consider a collision

$$\mathbf{S}_1^- + \mathbf{S}_2^- \underset{t=t_0}{\overset{Q_1}{\rightarrow}} \mathbf{S}_1^+ + \mathbf{S}_2^+. \tag{4.1}$$

Since we exclude the action of external forces, external moments, and nonkinetic degrees of freedom, the conservation laws read

$$\mathbf{p}_1^- + \mathbf{p}_2^- = \mathbf{p}_1^+ + \mathbf{p}_2^+, \tag{4.2}$$

$$\begin{aligned} &\not{s}_1^- + \mathbf{x}_1\times\mathbf{p}_1^- + \not{s}_2^- + \mathbf{x}_2\times\mathbf{p}_2^- \\ &\quad = \not{s}_1^+ + \mathbf{x}_1\times\mathbf{p}_1^+ + \not{s}_2^+ + \mathbf{x}_2\times\mathbf{p}_2^+, \end{aligned} \tag{4.3}$$

$$E_+^- + E_2^- = E_1^+ + E_2^+. \tag{4.4}$$

Of course, the mass m and the moment of inertia θ, as well as the shape of each body is the same before and after the collision; we say that the collision does not alter the bodies.

Our additional collision equations include the impact parameters. We suppose that:

(1) The component of the linear momentum of body 1 parallel to the tangent vector $\hat{u}_1$ is not changed by the collision:

$$\mathbf{p}_1^-\cdot\hat{u}_1 = \mathbf{p}_1^+\cdot\hat{u}_1. \tag{4.5}$$

(2) The angular momentum of body 1 around the impact point is not changed by the collision:

$$\not{s}_1^- - \mathbf{r}_1\times\mathbf{p}_1^- = \not{s}_1^+ - \mathbf{r}_1\times\mathbf{p}_1^+. \tag{4.6}$$

Using (4.5), we may write (4.6) as

$$\not{s}_1^- - \mathbf{b}_1\times\mathbf{p}_1^- = \not{s}_1^+ - \mathbf{b}_1\times\mathbf{p}_1^+, \tag{4.7}$$

or

$$\not{s}_1^- - \beta_1\mathbf{p}_1^-\cdot\hat{n}_1 = \not{s}_1^+ - \beta_1\mathbf{p}_1^+\cdot\hat{n}_1.$$

Notice that (4.5)–(4.7) too have the form of conservation equations

$$f(\mathbf{S}_i^-) = f(\mathbf{S}_i^+).$$

Relations (4.2)–(4.6) form a system of six equations for six unknown quantities $(\mathbf{p}_i^+, \not{s}_i^+)$. Equation (4.4) is quadratic, while all other equations are linear; one easily verifies that the linear system is not degenerate, and especially that (4.4) is not redundant. Therefore, at most two sets of states $\mathbf{S}_i^{\text{out}}$ can be solutions:

(a) the set $\mathbf{S}_i^{\text{out}} = \mathbf{S}_i^-$, in which case there occurs no collision at all;

(b) the set $\mathbf{S}_i^{\text{out}} = \mathbf{S}_i^+ \neq \mathbf{S}_i^-$, in which case there is a collision.

The explicit calculation of $\mathbf{S}_i^+$ is easy:

(1) From (4.2) and (4.5) follows

$$\mathbf{p}_2^-\cdot\hat{u}_2 = \mathbf{p}_2^+\cdot\hat{u}_2. \tag{4.8}$$

(2) Taking in (4.3) Q as the origin and using (4.6), we find also

$$\not{s}_2^- - \mathbf{r}_2\times\mathbf{p}_2^- = \not{s}_2^+ - \mathbf{r}_2\times\mathbf{p}_2^+. \tag{4.9}$$

(3) With the help of (4.5)–(4.9) and (4.2), the energy equation (4.4) becomes

$$\frac{1}{2D}(p_E^-)^2 = \frac{1}{2D}(p_E^+)^2, \tag{4.10}$$

where D is the "impact mass"

$$\frac{1}{D} \equiv \frac{1}{m_1} + \frac{1}{m_2} + \frac{b_1^2}{\theta_1} + \frac{b_2^2}{\theta_2} > 0 \tag{4.11}$$

and the Euler momentum

$$p_E \equiv D v_E, \tag{4.12}$$

$$v_E \equiv (\mathbf{v}_1 + \mathbf{b}_1 \times \omega_1)\cdot \hat{n}_1 + (\mathbf{v}_2 + \mathbf{b}_2 \times \omega_2)\cdot \hat{n}_2. \tag{4.13}$$

The scalar v_E, the "Euler velocity," is the normal relative velocity of the impact points Q_1 and Q_2. We notice that before the impact $(t < t_0)$,

$$v_E^- < 0, \tag{4.14a}$$

after the impact $(t > t_0)$,

$$v_E^+ > 0 \tag{4.14b}$$

because the bodies repell each other.

Using (4.14) and Eqs. (4.10)–(4.13), we find

$$p_E^+ = -p_E^- . \tag{4.15}$$

This equation (Euler, 1737) is the only one in the section expressing that the collision changed the states of the bodies; for case (a) we would find simply

$$p_E^{\text{out}} = -p_E^- .$$

Simple algebra then leads from (4.15) to the following equations:

$$\mathbf{p}_i^+ = \mathbf{p}_i^- - 2p_E^- \hat{n}_i, \tag{4.16a}$$

$$\mathscr{s}_i^+ = \mathscr{s}_i^- - 2p_E^- \beta_i \hat{e}. \tag{4.16b}$$

One sees that p_E^- is half the impulse transmitted by the impact, and that the lever directly influences the changes in linear and angular momentum,

$$\delta \mathscr{s}_i = \mathbf{b}_i \times \delta \mathbf{p}_i, \tag{4.17}$$

with the notation

$$\delta A_i \equiv A_i^+ - A_i^- . \tag{4.18}$$

Thus, the final states $(\mathbf{S}_1^+, \mathbf{S}_2^+)$ are entirely determined by the initial states $(\mathbf{S}_1^-, \mathbf{S}_2^-)$ and the impact parameters $(\mathbf{b}_1, \mathbf{b}_2)$.

B. The collision equations for velocities

Although the momenta are the canonical variables for describing a binary collision, we shall often use the velocities of the bodies. Therefore we express Eqs. (4.16) in terms of velocities:

$$\mathbf{v}_i^+ = \mathbf{v}_i^- - 2(D/m_i) v_E^- \hat{n}_i, \tag{4.19a}$$

$$\omega_i^+ = \omega_i^- - 2(D/\theta_i) v_E^- \beta_i \hat{e}. \tag{4.19b}$$

C. The collision matrix

With the help of the (formal) Euler collision matrix C_E, which operates on the "complete velocities," Eqs. (4.19) may be written as

$$\begin{pmatrix} \mathbf{V}_1^+ \\ \mathbf{V}_2^+ \end{pmatrix} = C_E \begin{pmatrix} \mathbf{V}_1^- \\ \mathbf{V}_2^- \end{pmatrix}. \tag{4.20}$$

Here

$$C_E \equiv I + \mathscr{C}_E, \quad I = \text{unit matrix}, \tag{4.21a}$$

$$\mathscr{C}_E \equiv \begin{pmatrix} \mathscr{C}_{11} & -\mathscr{C}_{12} \\ -\mathscr{C}_{21} & \mathscr{C}_{22} \end{pmatrix}, \tag{4.21b}$$

$$\mathscr{C}_{ij} \equiv \begin{pmatrix} -2(D/m_i)N & -2(D/m_i)\mathbf{b}_j \times \\ 2(D/\theta_i)\mathbf{b}_i \times & -2(D/\theta_i)\beta_i \beta_j \end{pmatrix}, \tag{4.21c}$$

where N is the projector onto the collision axis

$$N\mathbf{v} = \hat{n}_1(\hat{n}_1 \cdot \mathbf{v}). \tag{4.22}$$

This matrix is involutive,

$$C_E^2 = I. \tag{4.23}$$

Therefore, it has an inverse. Furthermore, it has negative determinant:

$$\det C_E = -1. \tag{4.24}$$

It follows that the equations expressing $\mathbf{S}^-$ in terms of $\mathbf{S}^+$ are of the same form.

Finally, diagonalization shows that C_E (resp. $\mathscr{C}_E$) has eigenvalues $+1$ (resp. 0) fivefold and -1 (resp. -2) singly; v_E is the "eigenvector" associated with the latter. This corresponds exactly to the series of hypotheses (4.2)–(4.6) together with (4.15).

D. Collision matrix and impact parameters

Since the impact parameters enter the collision equations (4.20) only through the collision matrix, one may ask whether this matrix fixes the impact parameters completely. The answer is provided by the solution of the equation:

$$C_E^A = C_E^B \tag{4.25}$$

with respect to β_i^B and $\hat{n}_i^B$, if β_i^A and $\hat{n}_i^A$ are known. From (4.21) follows

$$D^A N^A = D^B N^B$$

or

$$N^B = (D^A/D^B) N^A.$$

Since N^A and N^B are projectors, this implies

$$D^A = D^B, \tag{4.26a}$$

$$N^A = N^B, \tag{4.26b}$$

and, since $\hat{n}_1$ is a unit vector, (4.26b) becomes

$$\hat{n}_i^A = \sigma \hat{n}_i^B, \quad \sigma = \pm 1. \tag{4.27a}$$

From (4.21c) and (4.26a) follows

$$\mathbf{b}_i^A = \mathbf{b}_i^B, \tag{4.27b}$$

whence

$$\beta_i^A = \sigma \beta_i^B. \tag{4.27c}$$

This establishes

Proposition 2: Two collision matrices C_E^A and C_E^B are equal if and only if they refer to constellations either equivalent or antiequivalent.

This property will be essential in the next section.

V. COMPENSATING COLLISIONS

A. Requirements and definitions

Consider a collision (called in the following the *direct* collision)

$$\mathbf{S}_1^- + \mathbf{S}_2^- \xrightarrow{(l_i)} \mathbf{S}_1^+ + \mathbf{S}_2^+ . \tag{5.1}$$

We may view this collision as a process responsible for a displacement of two bodies in the space of states from states $\mathbf{S}_i^-$ to states $\mathbf{S}_i^+$. One may then look for collisions which compensate this "flow," either directly or by a cycle. We shall restrict ourselves to the first case and call the possible candidates "*compensating collisions.*"

Let us first try collisions of the form

$$\mathbf{S}_1^+ + \mathbf{S}_2^+ \rightarrow \mathbf{S}_1^- + \mathbf{S}_2^-, \tag{5.2}$$

with some convenient impact points Q_1^*, Q_2^*. Such collisions, if they exist, will be called *converse* to the direct collision under consideration.

We now ask: Given a direct collision, does there exist a converse collision? The answer is never. Given $\mathbf{S}_1^+$ and $\mathbf{S}_2^+$, the constellation of the collision is completely determined, and one has

$$v_E = v_E^+ > 0.$$

This makes an impact impossible [see relation (4.14)]. Because of this contradiction, we must weaken our requirements and define the inverse collision of (5.1) as

$$\mathbf{y}_1^+ + \mathbf{y}_2^+ \xrightarrow{l_1^*} \mathbf{y}_1^- + \mathbf{y}_2^- \tag{5.3}$$

or

$$\mathbf{V}_1^+ + \mathbf{V}_2^+ \xrightarrow{(\phi_1,\phi_2,\, l_1^*)} \mathbf{V}_1^- + \mathbf{V}_2^- .$$

Since we neglect the effects of all external fields on a collision, we need not specify where the collision occurs (in the vicinity of $\mathbf{x}_1^0, \mathbf{x}_2^0$). For definiteness we shall suppose that the impact point Q^* (in the plane) coincides with Q. Given a direct collision between two discs, an inverse collision does always exist; indeed, because there is no angular momentum transfer, we need substitute only

$$\mathbf{v}_1^{*-} = \mathbf{v}_1^+, \quad \mathbf{v}_2^{*-} = \mathbf{v}_2^+ .$$

In this degenerate case, ϕ_1 and ϕ_2 are irrelevant (see Fig. 2). But for bodies of arbitrary shape, this is not always possible.[5] As an example, consider a wedge at rest into which a disc collides (Fig. 3). One sees that no impact point is available to stop the wedge without deviating the disc or setting

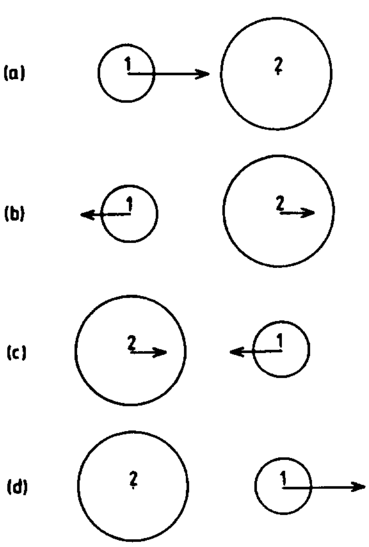

FIG. 2. Colliding rigid discs: (a) direct collision, incoming states, (b) direct collision, outgoing states, (c) inverse collision, incoming states, (d) inverse collision, outgoing states.

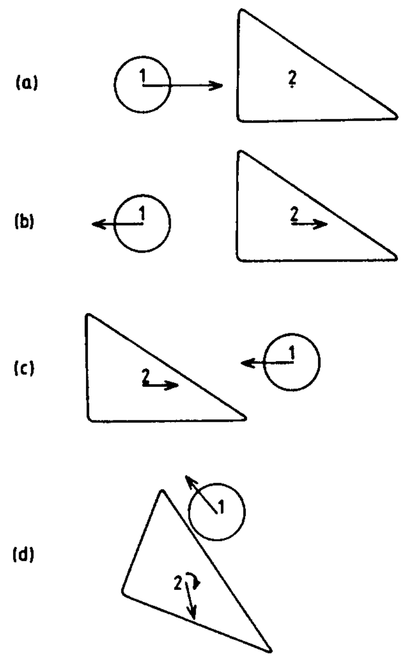

FIG. 3. Colliding arbitrary rigid bodies: (a) direct collision, incoming states, (b) direct collision, outgoing states, (c) incoming states for a presumed inverse collision, (d) outgoing states for the collision from (c).

the wedge into rotation: condition (5.3) cannot be fulfilled because of Eq. (4.17).

Therefore, we weaken our requirement further and demand a *reciprocal* collision of (5.1) only:

$$\mathbf{V}_1^+ + \mathbf{V}_2^+ \xrightarrow{(\phi_1^*,\phi_2^*,\, l_1^*)} \mathbf{V}_1^- + \mathbf{V}_2^-, \tag{5.4}$$

without any requirement as to the new constellation. This weakening is consistent since it does not affect the essential properties:

$$(\delta \mathbf{p}_i)^{\text{rec}} = -(\delta \mathbf{p}_i)^{\text{dir}}, \tag{5.5a}$$

$$(\delta s_i)^{\text{rec}} = -(\delta s_i)^{\text{dir}}. \tag{5.5b}$$

Definition (5.4) is the most general one compatible with (5.5).

An inverse collision is obviously also reciprocal; and clearly, (5.1) is also converse to (5.2), inverse to (5.3), and reciprocal to (5.4). Of course, none of these collisions are the time reversal of each other!

We shall now give a necessary and sufficient condition for the existence of a reciprocal collision to any given one.

B. Existence condition for a reciprocal collision

The direct collision (5.1) is described by Eqs. (4.19). The reciprocal collision (5.4) is described by similar equations, in which superscripts + and − have been interchanged. It follows from (4.20) and (4.23) that the reciprocal collision is characterized by the same matrix C_E as the direct collision. Therefore,

$$\beta_i^* = \sigma \beta_i, \tag{5.6a}$$

$$\hat{n}_i^* = \sigma \hat{n}_i, \tag{5.6b}$$

with $\sigma = \pm 1$. From this result and from definition (4.13), we derive

$$v_E^{*-} = \sigma v_E^+ .$$

In accordance with (3.4), we require $v_E^+ > 0$, $v_E^- < 0$. Hence

$$\sigma = -1. \tag{5.6c}$$

Thus we have proved

Theorem 1: Two collisions

$$\mathbf{V}_1^- + \mathbf{V}_2^- \rightarrow \mathbf{V}_1^+ + \mathbf{V}_2^+,$$

and

$$\mathbf{V}_1^{*-} + \mathbf{V}_2^{*-} \rightarrow \mathbf{V}_1^{*+} + \mathbf{V}_2^{*+}$$

are reciprocal to each other if and only if

(1) $\mathbf{V}_1^+ = \mathbf{V}_1^{*-}$ and $\mathbf{V}_2^+ = \mathbf{V}_2^{*-}$,

(2) their constellations are antiequivalent.

Since condition (5.6b) may always be satisfied by a proper choice of the bodies' orientations ϕ_i, the existence of a reciprocal collision depends only upon the existence of an antiequivalent constellation. In general, this condition cannot be fulfilled for bodies of arbitrary shape; in Sec. VI, we shall derive a sufficient condition for the existence of an antiequivalent point to *each* boundary point and thus for the existence of a reciprocal collision.

VI. SYMMETRIC BODIES

A. Geometry of one body

From now on, we shall impose a further restriction on the bodies: we shall demand that they possess a symmetry axis. That is,

(1) Under *reflection* in this axis, the boundary goes over into itself. We shall call such a body *geometrically symmetric*. Notice that in general such a body does *not* possess a symmetry center: in two dimensions, rotational symmetry of order 2 already insures the existence of such a center (and conversely); nor would such a symmetry help matters.

(2) We demand that the c.m. be on the symmetry axis; such a body will be called mechanically symmetric, or, for short, *symmetric*. For symmetric bodies, ψ will always be measured from the symmetry axis.

Proposition 3: If a body B is symmetric, the two boundary points $Q(\psi)$ and $Q(-\psi)$ are antiequivalent.

Proof: $r(\psi)$ is an even function of ψ.

Corollary 1: If B is symmetric, the boundary points $Q(0)$ and $Q(\pi)$ are indifferent.

Note:

—A body may have more than two indifferent points;

—Consider the class of all equivalent points; a point antiequivalent to one of them is antiequivalent to all of them; thus we may speak of the class of points antiequivalent to a class. There follows:

Corollary 2: If B is symmetric, the number of points in both classes is the same.

B. Two-body constellations

Consider a constellation (ϕ_1, ϕ_2, l_1) of two arbitrary symmetrical bodies (Fig. 4), together with the constellation that results from a (mirror) reflection in an arbitrary axis with direction ϕ_0, passing through the impact point Q. We shall denote by a superscript M all quantities referring to this image. Thus

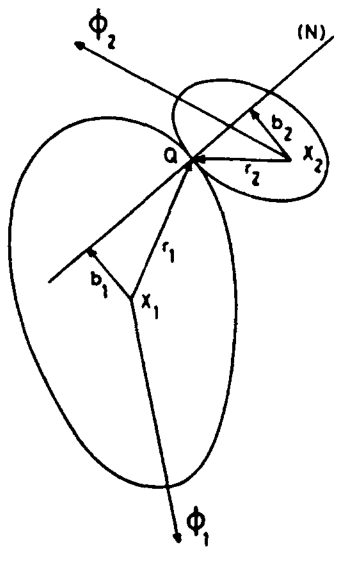

FIG. 4. Collision of two symmetric bodies: (N) collision axis, (Q) impact point.

$$Q^M = Q.$$

Obviously,

$$\psi_i^M = -\psi_i \quad \text{and} \quad \beta_i^M = -\beta_i.$$

This means that the mirror constellation is anticongruent to the direct one. Furthermore,

$$\phi_i^M = 2\phi_0 - \phi_i$$

since by construction $\phi_0^M = \phi_0$. This implies for the differentials

$$d\phi_i^M = -d\phi_i, \quad dl_i^M = -dl_1.$$

The result is summed up by:

Theorem 2: For each constellation (ϕ_1, ϕ_2, l_1) of two symmetrical bodies, there exists an infinite class of anticongruent constellations $(\phi_1^*, \phi_2^*, l_1^*)$.

These constellations form a one-parameter family. Furthermore,

$$dl_1^* = -dl_1, \quad d\phi_1^* = -d\phi_1, \quad d\phi_2^* = -d\phi_2.$$

Moreover, among the anticongruent constellations, there is one and only one antiequivalent to the direct constellation.

Corollary 1: For each constellation (ϕ_1, ϕ_2, l_1) of two symmetrical bodies, the class of anticongruent constellations $(\phi_1^*, \phi_2^*, l_1^*)$ has the same range as the class of congruent constellations $(\phi_1^=, \phi_2^=, l_1^=)$.

Proof: Compare with the Corollary of Proposition 1 [Eqs. (3.9)].

Corollary 2: The same relation holds when "congruent" is replaced by "equivalent" and "anticongruent" by "antiequivalent."

VII. PROSPECTIVE REMARKS

The properties established in the present paper suffice for a number of purposes, but the theory is not yet complete. A first question arises from the consideration of the conservation equation (4.2)–(4.6): Are the summational invariants of these binary collisions always linear combinations of the conserved quantities? There are reasons to believe so, but we have not yet completed a rigorous proof.

On the other hand, the sufficient condition presented in Sec. VII is not necessary. A theorem, proved by one of us (Y.E.), determines all possible conditions under which to each boundary point corresponds an antiequivalent one; the consequences of this theorem are under examination.

A more detailed discussion of the collision equation can be found in a previous report by one of us.[1]

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Classical mechanics of nonspherical bodies. II. Boltzmann equation and H-theorem in two dimensions

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An H-theorem is proved for a gas of two-dimensional rigid bodies which are not spherically symmetric but possess only a symmetry axis.

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I. INTRODUCTION

A. Introductory remarks

In a previous preprint,[1] a kinetic equation for two-dimensional noncircular rigid bodies was proposed. The purpose of this paper is to present an alternative derivation of this equation and to show that, under suitable restrictions, an H-theorem can be derived from the kinetic equation, without using the ergodic theory. But these restrictions do not affect the derivation of hydrodynamics.

All notions associated with binary collisions, which are needed in this article, were presented in the first paper of this series,[2] hereafter referred to as I. The notations, too, are the same as in I, and formulae from I will be referred to in the form (I.1.3).

B. Nature of the problem and aim of this paper

Attempts to generalize Boltzmann's equation to bodies with internal degrees of freedom have encountered a difficulty formulated first by Lorentz.[3] Lorentz noticed that the shape of a rigid body may be such that, in general, for a given collision

$$(\mathbf{v}_1^-,\omega_1^-)(\mathbf{v}_2^-,\omega_2^-)\rightarrow(\mathbf{v}_1^+,\omega_1^+)(\mathbf{v}_2^+,\omega_2^+)$$

the "compensating collision"

$$(\mathbf{v}_1^+,\omega_1^+)(\mathbf{v}_2^+,\omega_2^+)\rightarrow(\mathbf{v}_1^-,\omega_1^-)(\mathbf{v}_2^-,\omega_2^-)$$

does not exist. This argument may be circumvented by considering chains of collisions, which ultimately lead to the recurrence of the initial pair of states. In general, one must then use ergodic arguments. A detailed account of these questions may be found in the classical treatises of Boltzmann[4] himself and of Tolman[5]; Grad,[6] too, considers the hydrodynamics and the statistical mechanics of these systems.

In the framework of quantum mechanics, a similar problem has been studied by Stückelberg,[7] by Heitler,[8] and recently by Yang and Yang.[9]

The present approach rests on classical collision equations for binary eccentric collisions, found independently in 1737 by D. Bernoulli and Euler; more details are given in I, where references are quoted.

While completing this work, one of us (Y.E.) received a series of articles from Curtiss,[10] where a similar equation is proposed and used in three dimensions. But Curtiss, as his collision equation indicates, does not seem to know Euler's equations and theorem, which makes his argumentation less transparent and convincing. Furthermore, Curtiss subjects the bodies to the restriction of having a center of symmetry, while neither the binary collision formulae nor the kinetic equation need such an hypothesis. On the other hand, in two dimensions, this hypothesis is not adequate for the derivation of a H-theorem.

Finally, we note that the kinetic theory of gases with internal degrees of freedom has been the subject of many studies since the fundamental work of Wang-Chang and Uhlenbeck.[11,12]

C. Outline of the paper

In Sec. II, we introduce the one-body distribution function (Sec. IIA) and the corresponding Boltzmann equation (Sec. IIB). In Sec. III follows the calculation of macroscopic variables with a definition of moments (Sec. IIIA) and the main forms of collision integrals (Secs. IIIB and IIIC).

In Sec. IV, we restrict ourselves to axially (i.e., reflection) symmetric bodies (defined in Sec. VI of I). Then the symmetrization of collision integrals is carried out under some (restrictive) symmetry hypothesis on the microscopic variables (Secs. IVA, IVB, IVC). These symmetric collision integrals yield a proof of the H-theorem (Sec. IVD), for which one needs a distribution function that is an even function of the orientation of the body:

$$f(\mathbf{x},\phi,\mathbf{v},\omega,t)=f(\mathbf{x},-\phi,\mathbf{v},\omega,t).$$

An appendix contains a remark about odd functions of ϕ and their use for a possible H-theorem.

II. BOLTZMANN EQUATION

A. Distribution function

Since the state of a body is completely determined by the quantities $\mathbf{x}$, $\mathbf{v}$, ϕ, ω, we may consider a one-body distribution function

$$f(\mathbf{S},t)=f(\mathbf{x},\phi,\mathbf{v},\omega,t)$$

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and its time-evolution

$$d_t f \equiv \partial_t f + \mathbf{v}\cdot\partial_{\mathbf{x}} f + \omega\cdot\partial_\phi f + (1/m)\mathbf{F}\cdot\partial_{\mathbf{v}} f + (1/\theta)\mathscr{M}\cdot\partial_\omega f, \tag{2.1}$$

where $\mathbf{F}$ and $\mathscr{M}$ are given external fields. In the following, we shall often write $f(\mathbf{S})$ instead of $f(\mathbf{S}, t)$.

B. Boltzmann equation

In the framework of a low density approximation, one may look for an equation which describes the evolution of the one-body distribution function, in the form

$$d_t f(\mathbf{S}, t) = I_{\text{incr}}(\mathbf{S}, t) - I_{\text{decr}}(\mathbf{S}, t). \tag{2.2}$$

All approximations appear in the expressions for the integrals I_{incr} and I_{decr}, formed in terms of two one-body distribution functions. Since the derivation of an H-theorem as well as the identification of the hydrodynamic variables require a number of symmetrizations, it is indicated to write the collision integrals as symmetrically as possible. This will be done with the help of a redundant state $\mathbf{S}$ and an additional Dirac function.

The number of bodies leaving state $\mathbf{S}$ because of binary collisions can be written as

$$I_{\text{decr}}(\mathbf{S}, t) = \int\!\!\int\!\!\int f(\mathbf{S}_1^-) f(\mathbf{S}_2^-)\delta(\mathbf{S}_1^- - \mathbf{S}) \times K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1) dl_1 d\mathbf{S}_1^- d\mathbf{S}_2^-. \tag{2.3}$$

Here, l_1 refers to the boundary point of body 1 hit by body 2; $f(\mathbf{S}_1^-)$ and $f(\mathbf{S}_2^-)$ indicate that the rate of decrease is proportional to the number of bodies in states $\mathbf{S}_1^-$ and $\mathbf{S}_2^-$ (uncorrelated); integration on $\mathbf{S}_1^-$ and $\mathbf{S}_2^-$ takes into account all possible collisions; $\delta(\mathbf{S}_1^- - \mathbf{S})$ reflects the condition that one of the bodies leaves state $\mathbf{S}$; $K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1)$ is the kernel of the collision operator:

$$K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1) \equiv |v_{\mathrm{E}}|\delta(\mathbf{Q}_1 - \mathbf{Q}_2) \tag{2.4}$$

and depends on l_1 through v_{E}.

Obviously,

$$K(\mathbf{S}_1^+, \mathbf{S}_2^+, l_1) = K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1). \tag{2.5}$$

If we assume that

$$f(\mathbf{x}_i, \mathbf{y}_i, t) \simeq f(\mathbf{Q}_i, \mathbf{y}_i, t), \tag{2.6}$$

i.e., that the characteristic lengths of variation for the one-body distribution function are much greater than the body's size,[13] the spatial integrations become trivial:

$$I_{\text{decr}}(\mathbf{x}, \mathbf{y}, t) = \int\!\!\int\!\!\int f_1^- f_2^- \delta(\mathbf{y}_1^- - \mathbf{y})|v_{\mathrm{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-, \tag{2.7}$$

where $f_1^- = f(\mathbf{x}, \mathbf{y}_1^-, t)$.

In a "Stosszahlansatz"-like derivation, one may associate in (2.3):

$f(\mathbf{S}_1^-)dl_1$ with the target,

$f(\mathbf{S}_2^-)|v_{\mathrm{E}}|$ with the incoming flux.

Likewise, the number of bodies entering state $\mathbf{S}$ due to binary collisions is

$$I_{\text{incr}}(\mathbf{x}, \mathbf{y}, t) = \int\!\!\int\!\!\int f_1^- f_2^- \delta(\mathbf{S}_1^+ - \mathbf{S}) K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1)\, dl_1 d\mathbf{S}_1^- d\mathbf{S}_2^-. \tag{2.8}$$

This expression has the same status as (2.3) since the collision matrix is invertible (see I, Sec. IVC). Hence

$$\begin{aligned} d_t f(\mathbf{S}, t) &= \int\!\!\int\!\!\int f_1^- f_2^- [\delta(\mathbf{S}_1^+ - \mathbf{S}) - \delta(\mathbf{S}_1^- - \mathbf{S})] K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1)\, dl_1 d\mathbf{S}_1^- d\mathbf{S}_2^- \\ &= \int\!\!\int\!\!\int f_1^- f_2^- [\delta(\mathbf{y}_1^+ - \mathbf{y}) - \delta(\mathbf{y}_1^- - \mathbf{y})]|v_{\mathrm{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-. \end{aligned} \tag{2.9}$$

Because of the symmetry between 1 and 2, we may write

$$d_t f = \tfrac{1}{2}\int\!\!\int\!\!\int f_1^- f_2^- [\delta(\mathbf{y}_1^+ - \mathbf{y}) + \delta(\mathbf{y}_2^+ - \mathbf{y}) - \delta(\mathbf{y}_1^- - \mathbf{y}) - \delta(\mathbf{y}_2^- - \mathbf{y})]|v_{\mathrm{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-. \tag{2.10}$$

III. MACROSCOPIC VARIABLES

A. Moments

With any microscopic variable one may associate a macroscopic variable by taking its average over all states. Since all interactions are transmitted by contact (or possibly short range) interactions, it is convenient to single out the position dependence and write for any microscopic variable

$$A = A(\mathbf{x}, \mathbf{y}, t).$$

The macroscopic variable associated with A is the field

$$a(\mathbf{x}, t) = \int A(\mathbf{x}, \mathbf{y}, t) f(\mathbf{x}, \mathbf{y}, t)\, d\mathbf{y}, \tag{3.1}$$

for which an evolution equation is readily derived from the Boltzmann equation (4.9) and the evolution equation for $A(\mathbf{x}, \mathbf{y}, t)$

$$\frac{da}{dt} = \int \frac{dA}{dt} f\, d\mathbf{y} + C^a \tag{3.2}$$

with the *collision integral*

$$C^a(\mathbf{x}, t) = \int A(I_{\text{incr}} - I_{\text{decr}}) d\mathbf{y}. \tag{3.3}$$

The most useful of these moments will be the number density:

$$n(\mathbf{x}, t) \equiv \int 1 f(\mathbf{x}, \mathbf{y}, t) d\mathbf{y}. \tag{3.4}$$

One may then define the averages

$$\langle A \rangle(\mathbf{x}, t) = \frac{1}{n}\int A f\, d\mathbf{y} \tag{3.5}$$

and the fluxes

$$\mathbf{J}^a(\mathbf{x}, t) \equiv \int A(\mathbf{v} - \mathbf{u}) f\, d\mathbf{y}, \tag{3.6}$$

where $\mathbf{u} \equiv \langle \mathbf{v} \rangle$ is the mean velocity.

In this paper, we are not interested in the evolution equations themselves, and we shall not write them more explicitly. We only note that (3.2) may be rewritten as

$$\frac{d}{dt}\langle nA\rangle - n\langle d_t A\rangle = C^a \tag{3.7}$$

and focus our attention on the collision integral C^a.

B. Collision integrals

We must calculate

$$C^a = \int A\,(I_{\text{incr}} - I_{\text{decr}})d\mathbf{y}.$$

Inserting (2.9), we obtain

$$C^a = \int\int\int f(\mathbf{S}_1^-)f(\mathbf{S}_2^-)A(\mathbf{S})[\delta(\mathbf{S}_1^+ - \mathbf{S}) - \delta(\mathbf{S}_1^- - \mathbf{S})] \times K(\mathbf{S}_1^-, \mathbf{S}_2^-, l_1)dl_1 d\mathbf{S}_1^- d\mathbf{S}_2^-. \tag{3.8}$$

Provided that the approximation

$$A(\mathbf{x}, \mathbf{y}, t) \simeq A(\mathbf{Q}, \mathbf{y}, t) \tag{3.9}$$

holds, this relation may be written as

$$C^a = \int\int\int f_1^- f_2^- \delta A_1 |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-, \tag{3.10}$$

where

$$A_1^+ \equiv A(\mathbf{S}_1^+), \quad \text{etc.}$$
$$\delta A_i \equiv A_i^+ - A_i^-. \tag{3.11}$$

Relabeling $1 \rightleftarrows 2$, we also have

$$C^a = \int\int\int f_1^- f_2^- \delta A_2 |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-$$

and, taking half the sum of the two expressions,

$$C^a = \tfrac{1}{2}\int\int\int f_1^- f_2^- \Delta A\, |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-, \tag{3.12}$$

where ΔA is the collisional balance

$$\Delta A \equiv A_1^+ + A_2^+ - A_1^- - A_2^- = \delta A_1 + \delta A_2. \tag{3.13}$$

If $\Delta A = 0$, we say that A is a summational invariant of the collision. In this case, one has: $C^a = 0$. Hence, the principal hydrodynamic variables, namely the macroscopic averages of the collisional summational invariants, obey simple differential equations. But, for the nonhydrodynamic modes, there remains a special collisional source.

C. Other formulations

From (3.10) we derive also

$$\begin{aligned}
C^a &= \int\int\int f_1^- f_2^- A_1^+ |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \\
&\quad - \int\int\int f_1^- f_2^- A_1^- |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \\
&= \int\int\int f_1^- f_2^- A_1^+ |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \\
&\quad - \int\int\int f_1^+ f_2^+ A_1^+ |v_{\text{E}}| dl_1 d\mathbf{y}_1^+ d\mathbf{y}_2^+ \\
&= \int\int\int (f_1^- f_2^- - f_1^+ f_2^+) A_1^+ |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \\
&= \tfrac{1}{2}\int\int\int (f_1^- f_2^- - f_1^+ f_2^+)(A_1^+ + A_2^+) |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-.
\end{aligned} \tag{3.14}$$

Note that in general one is *not* allowed to symmetrize further by combining (3.14) with $(A_1^- + A_2^-)(f_1^- f_2^- - f_1^+ f_2^+)$ under the same integral, because there is no symmetry in the integrand between $\mathbf{S}_i^+$ and $\mathbf{S}_i^-$ and because time-reversal invariance is of no use here.

For proving an H-theorem with the use of only two (mutually) compensating collisions, one needs rather collision integrals of the form

$$\int\int\int (f_1 f_2 - \hat{f}_1\hat{f}_2)(A_1 + A_2 - \hat{A}_1 - \hat{A}_2)|v_{\text{E}}| dl_1 d\mathbf{y}_1 d\mathbf{y}_2, \tag{3.15}$$

where the symbol $\hat{}$ indicates an operation on the states. In order to carry through such an operation we shall make use of two additional restrictive assumptions, which we shall prove to be also sufficient. However, no such requirement is needed for Boltzmann's general proof of the H-theorem, which considers cycles of associated collisions but uses the ergodic theorem.

IV. SYMMETRICAL BODIES

In this section, as in Sec. VI of I, we apply the theory of the preceding sections to symmetric bodies. These bodies are defined as having a boundary symmetric under reflection in some mirror axis which passes through the center of mass. As indicated in I, we measure all angles ψ on a body's boundary from its symmetry axis.

A. General considerations

Consider the collision integral (3.10):

$$C^a = \int\int\int (A_1^+ - A_1^-) f_1^- f_2^- |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-. \tag{4.1}$$

With each constellation (ϕ_1, ϕ_2, l_1) we shall now associate an anticongruent constellation $(\phi_1^*, \phi_2^*, l_1^*)$. This association will be bijective, as suggested by the Corollaries of Theorem I.2, but there remains some ambiguity due to the free choice of the angle ϕ_0 for the mirror axis of Eq. (I.6.2). However, in all cases we have, according to the theorem

$$\begin{aligned}
C^a &= \int\int\int (A_1^{*+} - A_1^{*-}) f_1^{*-} f_2^{*-} |v_{\text{E}}^*| dl_1^* d\mathbf{y}_1^{*-} d\mathbf{y}_2^{*-} \\
&= \int\int\int (A_1^{*+} - A_1^{*-}) f_1^{*-} f_2^{*-} |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-.
\end{aligned} \tag{4.2}$$

Taking half the sum of (4.1) and (4.2), we find

$$C^a = \tfrac{1}{2}\int\int\int [(A_1^+ - A_1^-) f_1^- f_2^- + (A_1^{*+} - A_1^{*-}) \times f_1^{*-} f_2^{*-}] |v_{\text{E}}| dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-, \tag{4.3}$$

$$= \tfrac{1}{4}\int\int\int (\Delta A f_1^- f_2^- + \Delta A^* f_1^{*-} f_2^{*-})|v_{\text{E}}| \times dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^-. \tag{4.4}$$

Recall that

$$\begin{aligned}
&Q^* = Q, \qquad \phi_i^* = 2\phi_0 - \phi_i, \\
&\mathbf{v}_i^{*-} = \mathbf{v}_i^+, \qquad \mathbf{v}_i^{*+} = \mathbf{v}_i^-, \\
&\omega_i^{*-} = \omega_i^+, \qquad \omega_i^{*+} = \omega_i^-.
\end{aligned} \tag{4.5}$$

Two choices of anticongruent constellations are especially useful:

(1) The mirror axis is fixed in the space and is chosen to be the same for all constellations: this choice will be referred to as *uniform symmetrization*; since the direction of the normal is not invariant under this mirror reflection, the constellations related by (4.5) are generally only anticongruent rather than antiequivalent.

(2) The mirror axis is chosen parallel to the common tangent at the impact points in each constellation: this will be referred to as *constellational symmetrization*; then the constellations related by (4.5) are always antiequivalent.

Both possibilities will be pursued separately.

B. Uniform symmetrization

We use the mirror axis as the first coordinate axis in the plane:

$$\phi_* = 0. \tag{4.6}$$

Then, under the additional (necessary) assumption

$$A(\mathbf{x}, \phi, \mathbf{v}, \omega, t) = A(\mathbf{x}, -\phi, \mathbf{v}, \omega, t) \tag{4.7}$$

together with (3.9), we have

$$A_i^{*-} = A_i^{+}, \qquad A_i^{*+} = A_i^{-}; \tag{4.8}$$

thus,

$$\delta A_i^* = -\delta A_i, \tag{4.9a}$$

$$\Delta A^* = -\Delta A. \tag{4.9b}$$

Obviously (4.7) is a severe restriction. Then (4.4) becomes

$$C^a = \tfrac{1}{4}\int\!\!\int\!\!\int (A_1^+ + A_2^+ - A_1^- - A_2^-) \times (f_1^- f_2^- - f_1^{*-} f_2^{*-}) |v_{\mathrm{E}}|\, dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- . \tag{4.10}$$

Thus we have established an expression of the requested type (3.15), with the operator $\wedge$ acting on the states in a given collision:

$$\hat{\mathbf{S}}_i^+ \equiv \mathbf{S}_i^{*-} \quad \hat{\mathbf{S}}_i^- \equiv \mathbf{S}_i^{*+}.$$

C. Constellational symmetrization

The integrals in (4.3) involve a sum over all constellations. For any given direct collision we must relate $A_k^{*\pm}$ to $A_k^{\pm}$. This can be done in the form

$$A_k^{*+} = A_k^-, \qquad A_k^{*-} = A_k^+$$

provided that

$$A(\mathbf{x}, \mathbf{v}, 2\phi_0 - \phi, \omega, t) = A(\mathbf{x}, \mathbf{v}, \phi, \omega, t). \tag{4.11}$$

The latter condition must be fulfilled for any constellation, whatever the direction of the normal, $\hat{n}$, i.e., whatever the direction of the mirror axis ϕ_0. This in turn requires that A be independent of the orientation ϕ:

$$\partial A / \partial \phi = 0. \tag{4.12}$$

If this last condition is satisfied, it is obvious that

$$A(-\phi) = A(\phi).$$

This is the necessary and sufficient condition allowing uniform symmetrization. It follows that constellational symmetrization can be used under even stronger restrictions only. Therefore, we shall discuss it together with uniform symmetrization.

D. *H*-theorem using uniform symmetrization

A decisive feature of the classical Boltzmann equation is the existence of functionals H of the distribution function f, whose collision integral C^h is a semidefinite function of f. The proof of this property rests essentially on the form (3.15) of the collision integrals.

We have shown that a similar type of collision integral may be formed for symmetrical bodies using the uniform symmetrization hypothesis. Now we use expression (4.10) for finding all H-functions such that

$$\forall f, \qquad C^h \leqslant 0, \tag{4.13}$$

i.e.,

$$0 \geqslant \int\!\!\int\!\!\int (H_1^{*-} + H_2^{*-} - H_1^- - H_2^-)(f_1^- f_2^- - f_1^{*-} f_2^{*-}) \times |v_{\mathrm{E}}|\, dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- .$$

This requires that $(H_1^{*-} + H_2^{*-} - H_1^- - H_2^-)$ be a monotonic nonincreasing function of $(f_1^- f_2^- - f_1^{*-} f_2^{*-})$. This is tantamount to demanding that $(H_1^- + H_2^-)$ be a monotonic (increasing) function of $f_1^- f_2^-$, hence that H_1^- *be a monotonic function of* $\ln f_1^-$. An obvious simple choice is

$$H = \ln(f/f_0) \tag{4.14}$$

(with an arbitrary dimensional constant f_0), whence

$$C^h = \tfrac{1}{4}\int\!\!\int\!\!\int (f_1^- f_2^- - f_1^{*-} f_2^{*-}) \ln(f_1^{*-} f_2^{*-} / f_1^- f_2^-) \times |v_{\mathrm{E}}|\, dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- . \tag{4.15}$$

But, according to (4.15) and (4.7), such a substitution requires that

$$f(\mathbf{x}, \phi, \mathbf{v}, \omega, t) = f(\mathbf{x}, -\phi, \mathbf{v}, \omega, t). \tag{4.16}$$

The collision integrals may then be written

$$C^a = \tfrac{1}{4}\int\!\!\int\!\!\int (A_1^+ + A_2^+ - A_1^- - A_2^-)(f_1^- f_2^- - f_1^+ f_2^+) \times |v_{\mathrm{E}}|\, dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \tag{4.17}$$

just as for hard discs!

E. Future work

The derivation of macroscopic equations from the Boltzmann equation using the moments was outlined in Sec. III. The determination of the hydrodynamic equations becomes then possible from the moments of the summational invariants.

The equilibrium distribution too will be derived from the summational invariants.

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APPENDIX: EVEN AND ODD FUNCTIONS

In the framework of uniform symmetrization, it is interesting to consider also odd functions of the direction parameter:

$$A(\mathbf{x}, \mathbf{v}, -\phi, \omega, t) = -A(\mathbf{x}, \mathbf{v}, \phi, \omega, t). \tag{A1}$$

Then one has for a given collision

$$A_k^{*-} = -A_k^+, \quad A_k^{*+} = -A_k^-, \tag{A2}$$

whence

$$\begin{aligned} C^a &= \tfrac{1}{4}\iiint (A_1^+ + A_2^+ - A_1^- - A_2^-) \\ &\quad \times (f_1^- f_2^- + f_1^{*-} f_2^{*-}) |v_E| \, dl_1 d\mathbf{y}_1^- d\mathbf{y}_2^- \\ &= -\tfrac{1}{4}\iiiint (A_1^- + A_2^- + A_1^{*-} + A_2^{*-}) \\ &\quad \times (f_1^- f_2^- + f_1^{*-} f_2^{*-}) \\ &\quad \times |v_E| \, d_1 d\mathbf{y}_1^- d\mathbf{y}_2^- . \end{aligned} \tag{A3}$$

One may again try to derive an H-theorem from (A3). Using (A3) and the definite positivity of

$$f_1^- f_2^- + f_1^{*-} f_2^{*-},$$

the basic relation (4.13)

$$\forall f, \quad C^h \leqslant 0$$

goes over into the statement

$$\forall \text{ collisions}, \quad H_1^- + H_2^- + H_1^{*-} + H_2^{*-} \geqslant 0 \tag{A4}$$

$$\text{or} \quad H_1^+ + H_2^+ - H_1^- - H_2^- \leqslant 0.$$

This relation depends on the balance of H only, and is independent of the distribution functions f themselves. An H-theorem may be thus be derived only if one is able to find a microscopic variable H whose total value (in a pair) always decreases in a collision:

$$\Delta H \leqslant 0. \tag{A5}$$

As this seems very artificial, it will not be discussed further.

One may notice the opposition between (A4) and the usual derivations of H-theorem from "microscopic reversibility" (which is paralleled by our H-theorem in Sec. IVD).

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Time-dependent quadratic constants of motion, symmetries, and orbit equations for classical particle dynamical systems with time-dependent Kepler potentials

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It is shown there are only two classes of time-dependent Kepler potentials $[V_2 \equiv \lambda_0(at^2 + bt + c)^{-1/2}/r, (b^2 - 4ac \neq 0)$, and $V_3 \equiv \lambda_0(\alpha t + \beta)^{-1}/r]$ for which the associated classical dynamical equations will admit quadratic first integrals more general than quadratic functions of the angular momentum. In addition to the angular momentum the system defined by V_2 admits only a "generalized time-dependent energy integral," while the system defined by V_3 admits in addition to these a time-dependent vector first integral that is a generalization of the Laplace–Runge–Lenz vector constant of motion (associated with the time-independent Kepler system). For the V_3 system the time-dependent vector first integral is employed to obtain in a simple manner the orbit equations in completely integrated form. The complete group of (velocity-independent) symmetry mappings is obtained for each of these two classes of dynamical systems and used to show that the generalized energy integral is expressible as a Noether constant of motion.

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1. INTRODUCTION

We determine constants of the motion, symmetry mappings, and orbit equations for certain time-dependent central force dynamical systems based upon Lagrangians[1]

$$\mathscr{L} = \tfrac{1}{2}\delta_{ij}\dot{x}^i\dot{x}^j + \Phi(t)/r,$$
$$r^2 \equiv \delta_{ij}x^ix^j,\ i,j = 1,2,3, \tag{1.1}$$

with concomitant equations of motion

$$\ddot{x}^i + \Phi(t)x^i/r^3 = 0. \tag{1.2}$$

Such dynamical equations arise in a time-dependent Kepler system. The time-dependence for such a gravitational problem could occur due to time variation in the gravitational "constant" G, as suggested by Dirac,[2] or in a more usual situation due to time variation in the mass, as would occur in an accretion problem. Another possible physical situation leading to these dynamical equations arises in a Coulomb problem with variable charge.

We restrict ourselves to the determination of constants of motion of the form

$$I \equiv \tfrac{1}{2}M_{ij}(x,t)\dot{x}^i\dot{x}^j + J_i(x,t)\dot{x}^i + K(x,t), \quad M_{ij} = M_{ji}, \tag{1.3}$$

where it is noted that the coefficients are explicitly time dependent. The form (1.3) includes the well-known angular momentum linear first integrals

$$L_{ij} \equiv x^i\dot{x}^j - x^j\dot{x}^i, \tag{1.4}$$

which of course are constants of motion of (1.2) for arbitrary $\Phi(t)$.

For the time-independent case $\Phi(t) = \Phi_0 =$ const the dynamical system (1.2) admits the well-known Laplace–Runge–Lenz vector constant of motion[3]

$$\mathbf{A}_0 \equiv \Phi_0^{-1}(\mathbf{L}\times\mathbf{v}) + \mathbf{r}/r, \quad \mathbf{L} = \mathbf{r}\times\mathbf{v},$$
$$\mathbf{v} = d\mathbf{r}/dt, \tag{1.5}$$

and the energy integral

$$E_0 \equiv \tfrac{1}{2}\mathbf{v}\cdot\mathbf{v} - \Phi_0/r. \tag{1.6}$$

It is to be noted that E_0 and the components of $\mathbf{A}_0$ are also special cases of (1.3).

Unless indicated otherwise *in this paper we assume throughout that $\Phi(t)$ is not constant.*

We shall consider two methods for obtaining constants of motion of the type (1.3):

(i) Direct solution of the equation[4]

$$\dot{I} \overset{\circ}{=} 0. \tag{1.7}$$

[As is well known, the orbits for all central force dynamical systems are planar. Hence we obtain the solution of (1.7) in two dimensions and show how to extend the results to three dimensions.]

(ii) Techniques that require the determination of symmetry mappings of the dynamical systems of type (1.2). (For the sake of generality, since no additional complications are introduced, we treat this part of the problem in n dimensions.)

As a consequence of our analysis we find there are only two $\Phi(t)$ functions, referred to as $\Phi_2(t)$ [Eq. (2.64)] and $\Phi_3(t)$ [Eq. (2.66)], for which the respective dynamical systems (1.2) will admit quadratic first integrals (1.3) more general than quadratic functions of the angular momentum. We find for both Φ_2 and Φ_3 the dynamical system (1.2) admits a scalar quadratic first integral E [Eq. (2.86)]. In addition the dynamical system based upon Φ_3 will admit a vector constant of motion $\mathbf{A}$ (2.83) whose components are quadratic first integrals of the form (1.3). These scalar and vector constants of

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motion are explicitly time dependent and may be regarded as generalizations respectively of the energy E_0 (1.6) and Laplace–Runge–Lenz $\mathbf{A}_0$ (1.5) constants of motion associated with the time-independent Kepler problem.

The complete group of symmetries admitted by each of the dynamical equations (1.2) [regarded as n-dimensional] determined by Φ_2 and Φ_3, respectively, is obtained. These symmetries are based upon infinitesimal (velocity independent) mappings that are functions of x^i and t. From this analysis it is shown that the above-mentioned scalar quadratic first integrals for both the Φ_2 and Φ_3 cases can be formulated as Noether constants of motion.

For the Φ_3 case the components of the vector constant of motion $\mathbf{A}$ (2.83), mentioned above, are used to obtain in explicit finite form the orbits in plane polar coordinates of the dynamical equations (1.2). The orbits so obtained are classified according to a "generalized eccentricity" in a manner similar to that used in the usual time-independent Kepler problem.

2. CONSTANTS OF MOTION BY DIRECT SOLUTION

We now proceed with the direct method of determining the constants of motion (1.3) of the dynamical system (1.2). As mentioned in the Introduction it is sufficient to assume the motion is two dimensional ($n = 2$).

The conditions to determine the unknown coefficients M_{ij}, J_i, K of (1.3) are obtained by requiring that $\dot{I}$ vanish for the solutions of the dynamical system (1.2). From (1.3) we find[4]

$$\dot{I} \doteq \tfrac{1}{2}M_{ij,k}\dot{x}^i\dot{x}^j\dot{x}^k + (J_{i,j} + \tfrac{1}{2}M_{ij,t})\dot{x}^i\dot{x}^j + [J_{i,t} - (\Phi/r^3)M_{ij}x^j + K_{,i}]\dot{x}^i - (\Phi/r^3)J_i x^i + K_{,t} \doteq 0, \tag{2.1}$$

in which the $\ddot{x}$ terms have been eliminated by means of (1.2). Since (2.1) must hold identically in the $\dot{x}$'s we obtain after symmetrization the following conditions on M_{ij}, J_i, K:

$$M_{ij,k} + M_{jk,i} + M_{ki,j} = 0, \tag{2.2}$$

$$J_{i,j} + J_{j,i} = -M_{ij,t}, \tag{2.3}$$

$$K_{,i} = (\Phi/r^3)M_{ij}x^j - J_{i,t}, \tag{2.4}$$

$$K_{,t} = (\Phi/r^3)J_i x^i. \tag{2.5}$$

We consider first the solution of (2.2) for the functions $M_{ij}(x,t)$. For $n = 2$, the equations (2.2) take the form

$$M_{11,1} = 0, \tag{2.6}$$

$$M_{22,2} = 0, \tag{2.7}$$

$$M_{11,2} + 2M_{12,1} = 0, \tag{2.8}$$

$$M_{22,1} + 2M_{12,2} = 0. \tag{2.9}$$

By (2.6) and (2.7), respectively, we have

$$M_{11} = M_{11}(x^2,t), \tag{2.10}$$

$$M_{22} = M_{22}(x^1,t). \tag{2.11}$$

From the integrability condition on M_{12} [$M_{11,22} = M_{22,11}$] derived from (2.8) and (2.9), it is seen by use of (2.10) and (2.11) that

$$M_{11,22} = M_{22,11} \equiv 2\psi_0(t). \tag{2.12}$$

Hence from (2.12) it follows that

$$M_{11}(x^2,t) = \psi_0(t)(x^2)^2 + \psi_2(t)x^2 + \psi_3(t), \tag{2.13}$$

$$M_{22}(x^1,t) = \psi_0(t)(x^1)^2 + \psi_1(t)x^1 + \psi_4(t). \tag{2.14}$$

If we make use of (2.13) in (2.8) and (2.14) in (2.9) we obtain, respectively,

$$2M_{12,1} = -[2\psi_0(t)x^2 + \psi_2(t)], \tag{2.15}$$

$$2M_{12,2} = -[2\psi_0(t)x^1 + \psi_1(t)]. \tag{2.16}$$

From (2.15) and (2.16), respectively, we find

$$2M_{12} = -[2\psi_0 x^2 + \psi_2]x^1 + \sigma_1(x^2,t), \tag{2.17}$$

$$2M_{12} = -[2\psi_0 x^1 + \psi_1]x^2 + \sigma_2(x^1,t). \tag{2.18}$$

By comparison of (2.17) and (2.18) we may write

$$\psi_2(t)x^1 + \sigma_2(x^1,t) = \psi_1(t)x^2 + \sigma_1(x^2,t) \equiv \mu(t). \tag{2.19}$$

It follows from (2.19) and either of (2.17) or (2.18) that

$$M_{12} = -\psi_0(t)x^1x^2 - \tfrac{1}{2}\psi_2(t)x^1 - \tfrac{1}{2}\psi_1(t)x^2 + \tfrac{1}{2}\mu(t). \tag{2.20}$$

Hence this solution of (2.2) for the M_{ij} is given by Eqs. (2.13), (2.14), and (2.20).

We consider next (2.3) to determine the functions $J_i(x,t)$. Use of (2.13), (2.14), and (2.20) in (2.3) gives

$$2J_{1,1} = -[\psi_0'(x^2)^2 + \psi_2'x^2 + \psi_3'], \tag{2.21}$$

$$2J_{2,2} = -[\psi_0'(x^1)^2 + \psi_1'x^1 + \psi_4'], \tag{2.22}$$

$$J_{1,2} + J_{2,1} = \psi_0'x^1x^2 + \tfrac{1}{2}\psi_2'x^1 + \tfrac{1}{2}\psi_1'x^2 - \tfrac{1}{2}\mu'. \tag{2.23}$$

Integration of (2.21) and (2.22) gives, respectively,

$$2J_1 = -x^1[\psi_0'(x^2)^2 + \psi_2'x^2 + \psi_3'] + \tau_1(x^2,t), \tag{2.24}$$

$$2J_2 = -x^2[\psi_0'(x^1)^2 + \psi_1'x^1 + \psi_4'] + \tau_2(x^1,t). \tag{2.25}$$

Hence from (2.24), (2.25), and (2.23) it follows that

$$6\psi_0'x^1x^2 + 2\psi_2'x^1 + 2\psi_1'x^2 - \tau_{1,2} - \tau_{2,1} - \mu' = 0. \tag{2.26}$$

By forming the second derivative of (2.26) with respect to x^1 and x^2 we find that

$$\psi_0(t) = a_0 = \text{const}. \tag{2.27}$$

Substitution of (2.27) into (2.26) followed by differentiation of the resulting equation gives

$$2\psi_2' - \tau_{2,11} = 0. \tag{2.28}$$

From (2.28) it follows that

$$\tau_2(x^1,t) = \psi_2'(x^1)^2 + \psi_5(t)x^1 + \psi_6(t). \tag{2.29}$$

Use of (2.29) and (2.27) in (2.26) followed by integration with respect to x^2 gives

$$\tau_1(x^2,t) = \psi_1'(x^2)^2 - (\psi_5 + \mu')x^2 + \psi_7(t). \tag{2.30}$$

Finally use of (2.29) and (2.30) in (2.24) and (2.25) gives

$$J_1 = -\tfrac{1}{2}x^1(\psi_2'x^2 + \psi_3') + \tfrac{1}{2}\psi_1'(x^2)^2 - \tfrac{1}{2}(\psi_5 + \mu')x^2 + \tfrac{1}{2}\psi_7, \tag{2.31}$$

$$J_2 = -\tfrac{1}{2}x^2(\psi_1'x^1 + \psi_4') + \tfrac{1}{2}\psi_2'(x^1)^2 + \tfrac{1}{2}\psi_5 x^1 + \tfrac{1}{2}\psi_6. \tag{2.32}$$

There remains the determination of the function K. From (2.4) the integrability condition $K_{,12} = K_{,21}$ can be expressed in the form

$$r^2\Phi\,[M_{11,2}x^1 + M_{12,2}x^2 - M_{12,1}x^1 - M_{22,1}x^2] - 3\Phi\,[M_{11}x^1x^2 + M_{12}(x^2)^2 - M_{12}(x^1)^2 - M_{22}x^1x^2] - r^5[J_{1,2t} - J_{2,1t}] = 0. \quad (2.33)$$

From (2.13), (2.14), (2.20), (2.31), and (2.32) it is seen that the bracketed expressions in (2.33) are polynomials in x^1, x^2. Since $n > 1$ the term r^5 is an irrational function of x^1, x^2. Hence it follows that

$$J_{1,2t} - J_{2,1t} = 0. \quad (2.34)$$

If (2.34) along with (2.13) and (2.14) are used in (2.33), we obtain by a straightforward calculation

$$2(\psi_4 - \psi_3)x^1x^2 + \mu[(x^1)^2 - (x^2)^2] = 0, \quad (2.35)$$

which implies

$$\mu = 0, \quad \psi_3 = \psi_4. \quad (2.36)$$

By the use of (2.31), (2.32), (2.34), and (2.36) we obtain

$$\psi_2'' = 0, \quad \psi_1'' = 0, \quad \psi_5 = a_5 = \text{const}. \quad (2.37)$$

We consider now the remaining integrability conditions

$$K_{,t1} = K_{,1t}, \quad (2.38)$$

$$K_{,t2} = K_{,2t}, \quad (2.39)$$

which must be satisfied. The derivative $K_{,t2}$ is calculated by means of (2.5), (2.31), (2.32), (2.36), and (2.37), and the derivative $K_{,2t}$ is calculated by means of (2.4), (2.14), (2.20), (2.32), and (2.37). If the expressions so obtained are used in (2.39) the resulting equation reduces to

$$\Phi' r^2[-\psi_2(x^1)^2 + \psi_1x^1x^2 + 2\psi_3x^2] + r^5(\psi_3'''x^2 - \psi_6'') + 3\Phi x^2(\psi_7x^1 + \psi_6x^2) + \Phi r^2[-\psi_2'(x^1)^2 + \psi_1'x^1x^2 + \psi_3'x^2 - \psi_6] = 0. \quad (2.40)$$

Inspection of (2.40) implies

$$\psi_3''' = 0, \quad \psi_6'' = 0. \quad (2.41)$$

Equation (2.40) reduces by use of (2.41) to a polynomial in x^1 and x^2. This leads to the conditions

$$2\psi_3\Phi' + \psi_3'\Phi = 0, \quad (2.42)$$

$$\psi_2\Phi' + \psi_2'\Phi = 0, \quad (2.43)$$

$$\psi_1\Phi' + \psi_1'\Phi = 0, \quad (2.44)$$

$$\psi_6 = 0, \quad \psi_7 = 0. \quad (2.45)$$

We summarize in the list below the previously obtained conditions on the various ψ's and μ [refer to (2.36), (2.37), (2.41), (2.45)] along with the restrictions derived by integrating (2.42)–(2.44).

$$\psi_0 = a_0, \quad (2.46)$$

$$\psi_3 = \psi_4, \quad (2.47)$$

$$\psi_5 = a_5, \quad (2.48)$$

$$\psi_6 = \psi_7 = 0, \quad (2.49)$$

$$\mu = 0, \quad (2.50)$$

$$\psi_2'' = 0, \quad (2.51)$$

$$\psi_3''' = 0, \quad (2.52)$$

$$\psi_1'' = 0, \quad (2.53)$$

$$\Phi\psi_2 = k_2, \quad (2.54)$$

$$\Phi^2\psi_3 = k_3, \quad (2.55)$$

$$\Phi\psi_1 = k_1, \quad (2.56)$$

where the a's and k's are arbitrary constants.

Before continuing with the integration of (2.4) and (2.5) to obtain K we use (2.46)–(2.50) to simplify the expressions for M_{ij} [refer to (2.13), (2.14), (2.20)] and J_i [refer to (2.31), (2.32)].

$$M_{11} = a_0(x^2)^2 + \psi_2x^2 + \psi_3, \quad (2.57)$$

$$M_{12} = -a_0x^1x^2 - \tfrac{1}{2}\psi_2x^1 - \tfrac{1}{2}\psi_1x^2, \quad (2.58)$$

$$M_{22} = a_0(x^1)^2 + \psi_1x^1 + \psi_3, \quad (2.59)$$

$$J_1 = -\tfrac{1}{2}\psi_2x^1x^2 + \tfrac{1}{2}\psi_1'(x^2)^2 - \tfrac{1}{2}\psi_3'x^1 - \tfrac{1}{2}a_5x^2, \quad (2.60)$$

$$J_2 = -\tfrac{1}{2}\psi_1'x^1x^2 + \tfrac{1}{2}\psi_2'(x^1)^2 - \tfrac{1}{2}\psi_3'x^2 + \tfrac{1}{2}a_5x^1. \quad (2.61)$$

The various conditions under which (2.51)–(2.56) will be consistent leads to the following three cases:

Case 1:

$$\Phi(t) = \Phi_1(t) = \text{arbitrary } (\neq \text{const}), \quad (2.62)$$

$$\psi_1 = \psi_2 = \psi_3 = 0; \quad k_1 = k_2 = k_3 = 0. \quad (2.63)$$

Case 2:

$$\Phi(t) = \Phi_2(t) \equiv \lambda_0(at^2 + bt + c)^{-1/2}, \quad a,b,c,\lambda_0 = \text{const}, \; b^2 - 4ac \neq 0, \; \lambda_0 \neq 0, \quad (2.64)$$

$$\psi_1 = \psi_2 = k_1 = k_2 = 0;$$

$$\psi_3 = k_3\lambda_0^{-2}(at^2 + bt + c), \quad k_3 = \text{const} \neq 0. \quad (2.65)$$

Case 3:

$$\Phi(t) = \Phi_3(t) = \lambda_0(\alpha t + \beta)^{-1}, \quad \lambda_0 \neq 0, \; \alpha \neq 0, \quad (2.66)$$

$$\psi_1 = k_1\lambda_0^{-1}(\alpha t + \beta); \quad \psi_2 = k_2\lambda_0^{-1}(\alpha t + \beta);$$

$$\psi_3 = k_3\lambda_0^{-2}(\alpha t + \beta)^2,$$

$$\alpha,\beta,\lambda_0,k_1,k_2,k_3 = \text{const}. \quad (2.67)$$

We now consider the analysis of the above three cases.

Analysis of Case 1

In Case 1 [$\Phi_1(t)$ arbitrary] use of (2.63) in (2.57)–(2.61) gives

$$M_{11} = a_0(x^2)^2, \quad M_{12} = -a_0x^1x^2, \quad M_{22} = a_0(x^1)^2, \quad J_1 = -\tfrac{1}{2}a_5x^2, \quad J_2 = \tfrac{1}{2}a_5x^1. \quad (2.68)$$

Use of (2.68) in (2.4) and (2.5) leads to $K = K_0 = \text{const}$, which may be dropped. With these values of M_{ij} and J_i so obtained it follows from (1.3) that

$$I_1 = \tfrac{1}{2}a_0L^2 + \tfrac{1}{2}a_5L, \quad L \equiv x^1\dot{x}^2 - x^2\dot{x}^1, \quad (2.69)$$

where L is the angular momentum.

As mentioned in the Introduction it is well known that angular momentum is a constant of motion for every dynamical system (1.2) [that is, for arbitrary $\Phi_1(t)$]. Since a_0 and a_5

are arbitrary constants we find that the *only common linear first integral admitted by every* dynamical system (1.2) is angular momentum; likewise the *only common quadratic first integral admitted by every* dynamical system (1.2) is a quadratic function of the angular momentum.

Analysis of Case 2

Use of (2.64) and (2.65) in (2.57)–(2.61) gives

$$M_{ij} = a_0(r^2\delta_{ij} - x^i x^j) + \psi_3\delta_{ij}, \qquad (2.70)$$

$$J_1 = -\tfrac{1}{2}(\psi_3' x^1 + a_5 x^2),$$
$$J_2 = -\tfrac{1}{2}(\psi_3' x^2 - a_5 x^1). \qquad (2.71)$$

By use of (2.70) and (2.71) in (2.4) and (2.5) we obtain upon integration

$$K = ak_3 r^2/(2\lambda_0^2) - \psi_3\Phi_2/r. \qquad (2.72)$$

Use of (2.70), (2.71), and (2.72) in (1.3) leads to the constant of motion I_2,

$$I_2 = \tfrac{1}{2}a_0 L^2 + \tfrac{1}{2}a_5 L + (k_3/\lambda_0^2)E_2, \qquad (2.73)$$

where

$$E_2 \equiv (at^2 + bt + c)\left[\frac{(\dot{x}^1)^2 + (\dot{x}^2)^2}{2} - \frac{\lambda_0}{r(at^2 + bt + c)^{1/2}}\right] - \frac{(2at + b)}{\lambda_0^2}(x^1\dot{x}^1 + x^2\dot{x}^2) + \frac{ar^2}{2}. \qquad (2.74)$$

Since L is a constant of motion it follows from (2.73) that E_2 is a constant of motion.

In terms of Φ_2 [refer to (2.64)] the constant of motion E_2 may be expressed in the alternative form

$$E_2 = \lambda_0^2\left[\frac{1}{(\Phi_2)^2}\left(\frac{\mathbf{v}\cdot\mathbf{v}}{2} - \frac{\Phi_2}{r}\right) - \frac{1}{2}\frac{d}{dt}\left(\frac{1}{\Phi_2}\right)^2 \mathbf{r}\cdot\mathbf{v} + \frac{d^2}{dt^2}\left(\frac{1}{\Phi_2}\right)^2\frac{r^2}{4}\right]. \qquad (2.75)$$

From (2.75) we note if $\Phi_2 = \Phi_0 = \text{const}$ [so that the dynamical system (1.2) reduces to the time-independent case] then E_2 reduces to E_0 [Eq. (1.6)], the time-independent energy integral.

Analysis of Case 3

If we make use of (2.66) and (2.67) in (2.57)–(2.61) and use the resulting M_{ij} and J_i in the K equations (2.4), (2.5), we find by integration

$$K = \frac{k_3\alpha^2 r^2}{2\lambda_0^2} - \frac{k_3(\alpha t + \beta)}{\lambda_0 r} - \frac{k_1 x^1 + k_2 x^2}{2r}. \qquad (2.76)$$

Use of (2.57)–(2.61) [with the appropriate ψ's given by (2.67)] and (2.76) in (1.3) gives the constant of motion I_3

$$I_3 = \tfrac{1}{2}a_0 L^2 + \tfrac{1}{2}a_5 L + \tfrac{1}{2}k_1 A_1 + \tfrac{1}{2}k_2 A_2 + (k_3/\lambda_0^2)E_3, \qquad (2.77)$$

where

$$A_1 \equiv \frac{L}{\lambda_0}[(\alpha t + \beta)\dot{x}^2 - \alpha x^2] - \frac{x^1}{r} \overset{\circ}{=} k_x, \qquad (2.78)$$

$$A_2 \equiv \frac{L}{\lambda_0}[-(\alpha t + \beta)\dot{x}^1 + \alpha x^1] - \frac{x^2}{r} \overset{\circ}{=} k_y, \qquad (2.79)$$

$$E_3 \equiv (\alpha t + \beta)^2\left[\frac{(\dot{x}^1)^2 + (\dot{x}^2)^2}{2} - \frac{\lambda_0}{r(\alpha t + \beta)}\right] - \alpha(\alpha t + \beta)(x^1\dot{x}^1 + x^2\dot{x}^2) + \frac{\alpha^2 r^2}{2} \overset{\circ}{=} k^*. \qquad (2.80)$$

Since a_0, a_5, k_1, k_2, and k_3 are arbitrary constants *it follows in addition to the angular momentum L that A_1, A_2, and E_3 are constants of motion* [which have the respective values k_x, k_y, and k^* on a dynamical path as indicated in (2.78)–(2.80)].

When expressed in terms of Φ_3 given by (2.66) the constant of motion E_3 may be given the form

$$E_3 = \lambda_0^2\left[\frac{1}{(\Phi_3)^2}\left(\frac{\mathbf{v}\cdot\mathbf{v}}{2} - \frac{\Phi_3}{r}\right) - \frac{1}{2}\frac{d}{dt}\left(\frac{1}{\Phi_3}\right)^2 \mathbf{r}\cdot\mathbf{v} + \frac{d^2}{dt^2}\left(\frac{1}{\Phi_3}\right)^2\frac{r^2}{4}\right]. \qquad (2.81)$$

The constants of motion A_1 and A_2 [refer to (2.78) and (2.79)] are components of a vector

$$\mathbf{A} = \hat{i}_1 A_1 + \hat{i}_2 A_2. \qquad (2.82)$$

This vector $\mathbf{A}$ can be expressed in the form

$$\mathbf{A} = \frac{(\alpha t + \beta)}{\lambda_0}(\mathbf{v}\times\mathbf{L}) - \frac{\alpha}{\lambda_0}(\mathbf{r}\times\mathbf{L}) - \frac{\mathbf{r}}{r}, \quad \mathbf{v} \equiv \frac{d\mathbf{r}}{dt}. \qquad (2.83)$$

If $\mathbf{r}$, $\mathbf{v}$, and $\mathbf{L}$ are considered as three-dimensional vectors, then the three-dimensional vector $\mathbf{A}$ of the form (2.83) will be a constant of motion of the corresponding three-dimensional system (1.2). This is easily verified by showing $d\mathbf{A}/dt \overset{\circ}{=} 0$ [with the aid of (1.2)].

The following functional dependence may be shown to exist between the constants of motion $\mathbf{A}$, $\mathbf{E}_3$, and $\mathbf{L}$:

$$2(\mathbf{L}\cdot\mathbf{L})E_3 + \lambda_0^2 = \lambda_0^2\mathbf{A}\cdot\mathbf{A}. \qquad (2.84)$$

Equation (2.84) holds in either two or three dimensions. On a dynamical path (which is assumed to be in the x–y plane), (2.84) takes the form

$$2l_0^2 k^* + \lambda_0^2 = \lambda_0^2(k_x^2 + k_y^2), \qquad (2.85)$$

where $l_0^2 \overset{\circ}{=} \mathbf{L}\cdot\mathbf{L}$.

If in Φ_3 (2.66) we consider $\alpha = 0$ [in which case $\Phi_3(t) = \Phi_0 = \text{const}$, and the dynamical equation (1.2) reduces to the *time-independent* equation of motion],[5] then the time-dependent constant of motion E_3 (2.81) reduces, within a constant factor, to the time-independent energy integral E_0 (1.6), and the time-dependent vector constant of motion $\mathbf{A}$ (2.83) reduces to the time-independent Laplace–Runge–Lenz vector constant of motion $\mathbf{A}_0$ (1.5).

We summarize the results of this section in the following theorem and corollaries.

Theorem 2.1: For an explicitly time-dependent central force dynamical system in two or three dimensional Euclidean space with Lagrangian

$$\mathscr{L} \equiv \tfrac{1}{2}\delta_{ij}\dot{x}^i\dot{x}^j + \Phi(t)/r, \quad r^2 \equiv \delta_{ij}x^i x^i, \qquad (1.1)'$$

and with associated dynamical equation

$$\ddot{x}^i + \Phi(t)x^i/r^3 = 0: \qquad (1.2)'$$

a) The only common linear first integral admitted by every [$\Phi(t)$ arbitrary] time-dependent dynamical system (1.2) is the angular momentum $\mathbf{L} \equiv \mathbf{r} \times \mathbf{v} (\mathbf{v} = d\mathbf{r}/dt)$.

b) The only common quadratic first integral admitted by every [$\Phi(t)$ arbitrary] time-dependent dynamical system (1.2)′ is a quadratic function of the angular momentum.

c) For an explicitly time-dependent dynamical system of the form (1.2)′ to admit a quadratic first integral in addition to a quadratic function of the angular momentum, the function $\Phi(t)$ must be either of the form

$$\Phi(t) = \Phi_2 \equiv \frac{\lambda_0}{(at^2+bt+c)^{1/2}}, \quad a,b,c,\lambda_0 = \text{const}, \ \lambda_0 \neq 0, \ b^2 - 4ac \neq 0, \tag{2.64$'$}$$

or of the form

$$\Phi(t) = \Phi_3 \equiv \frac{\lambda_0}{\alpha t + \beta}, \quad \lambda_0 \neq 0, \ \alpha \neq 0. \tag{2.66$'$}$$

d) For $\Phi(t) = \Phi_2$ or Φ_3 the dynamical system (1.2)′ will admit the scalar quadratic first integral [refer to (2.75) and (2.81)]

$$E \equiv \lambda_0^2 \Big[\Phi^{-2} \Big(\tfrac{1}{2} \mathbf{v}\cdot\mathbf{v} - \frac{\Phi}{r} \Big) - \frac{1}{2} \frac{d}{dt} (\Phi^{-2}) \mathbf{r}\cdot\mathbf{v} + \frac{d^2}{dt^2} (\Phi^{-2}) \frac{r^2}{4} \Big]. \tag{2.86}$$

e) For $\Phi(t) = \Phi_3$ the dynamical system (1.2)′ will admit besides E the additional vector quadratic first integral

$$\mathbf{A} \equiv \frac{(\alpha t + \beta)}{\lambda_0} (\mathbf{v} \times \mathbf{L}) - \frac{\alpha}{\lambda_0} (\mathbf{r} \times \mathbf{L}) - \frac{\mathbf{r}}{r}, \quad \mathbf{v} \equiv \frac{d\mathbf{r}}{dt}. \tag{2.83$'$}$$

Corollary 2.1: If the dynamical system (1.1), (1.2) is regarded as n dimensional ($i = 1,...,n$) then Theorem 2.1(d) is valid in n dimensions.

Corollary 2.2: For the $\Phi = \Phi_3$ case the first integrals **E**,**A**, and **L** are functionally related in that

$$2(\mathbf{L}\cdot\mathbf{L})E + \lambda_0^2 = \lambda_0^2 \mathbf{A}\cdot\mathbf{A}. \tag{2.84$'$}$$

Remark 2.1: In the limiting case of $\Phi(t) = \Phi_0 = \text{const}$ for which (1.2)′ reduces to a dynamical system with no explicit time dependence, the first integral E (2.86) reduces to E_0, the energy integral, and $\mathbf{A}$ (2.83)′ reduces to $\mathbf{A}_0$, the Laplace–Runge–Lenz vector first integral.

3. SYMMETRY MAPPINGS OF THE DYNAMICAL EQUATION (1.2)

It is of interest to determine to what extent the constants of motion derived in the previous section can be obtained as concomitants of infinitesimal symmetry mappings admitted by the equations of motion (1.2). We shall base this symmetry analysis upon deformations of the type[6]

$$\bar{x}^i = x^i + \delta x^i, \quad \delta x^i \equiv \xi^i(x,t)\delta a, \tag{3.1}$$

$$\bar{t} = t + \delta t, \quad \delta t \equiv \xi^0(x,t)\delta a. \tag{3.2}$$

The symmetries admitted by the dynamical systems (1.2) will in general depend upon the form of the function $\Phi(t)$. Our primary interest is to determine what symmetries are admitted by the dynamical systems that correspond to the three cases for $\Phi(t)$ obtained in Sec. 2. However, for generality we shall first determine all dynamical systems of the type (1.2) that admit symmetries based upon mappings of the form (3.1) and (3.2).

It is well known that for arbitrary $\Phi(t)$ the central force dynamical systems (1.2) will admit rotational symmetry (with concomitant angular momentum constant of motion). We shall determine those (nonconstant) $\Phi(t)$ whose corresponding dynamical systems admit symmetries in addition to rotations, and in the process obtain as subcases the symmetries for those particular dynamical systems based upon Φ_1, Φ_2, and Φ_3 considered in Sec. 2.

Based upon the above-mentioned mappings (3.1) and (3.2) it follows to within first order in δa that[7]

$$\delta \dot{x}^i \equiv \frac{d\bar{x}^i}{d\bar{t}} - \frac{dx^i}{dt} = (\dot{\xi}^i - \dot{x}^i \dot{\xi}^0)\delta a, \tag{3.3}$$

$$\delta \ddot{x}^i \equiv \frac{d^2\bar{x}^i}{d\bar{t}^2} - \frac{d^2 x^i}{dt^2} = (\ddot{\xi}^i - \dot{x}^i \ddot{\xi}^0 - 2\ddot{x}^i \dot{\xi}^0)\delta a. \tag{3.4}$$

With use of the definitions (3.1)–(3.4) the deformation of any function $F(\ddot{x},\dot{x},x,t)$ is determined by the formula

$$\delta F \equiv \frac{\partial F}{\partial \ddot{x}^i} \delta \ddot{x}^i + \frac{\partial F}{\partial \dot{x}^i} \delta \dot{x}^i + \frac{\partial F}{\partial x^i} \delta x^i + \frac{\partial F}{\partial t} \delta t. \tag{3.5}$$

The symmetry equations that determine those ξ^i,ξ^0 that define the symmetry mappings (3.1), (3.2) of some dynamical equations E^i are obtained from the requirement that $\delta E^i = 0$ whenever $E^i = 0$. Such symmetries will contain as special cases the more familiar Noether symmetries.[8]

For a dynamical system in an Euclidean configuration space of n dimensions referred to rectangular coordinates with Lagrangian $\mathscr{L} = \frac{1}{2}\delta_{ij}\dot{x}^i\dot{x}^j - V(x,t)$ this procedure leads to symmetry mapping functions ξ^i,ξ^0 of the form[7]

$$\xi^i = A_j^i(t) x^j x^i + B_j^i(t) x^j + C^i(t), \tag{3.6}$$

$$\xi^0 = A_j(t) x^j + B(t). \tag{3.7}$$

The functions $A_j(t)$ and $B(t)$ are to be determined as solutions of the equations

$$A_k V_{,k} \delta^i_m + 2A_m V_{,i} - (A_k'' x^k + B'')\delta^i_m + 2(A_m'' x^i + A_k'' x^k \delta^i_m + B_m^{i\prime}) = 0, \tag{3.8}$$

$$\begin{aligned} A_m''' x^m x^i &+ B_m^{i\prime\prime} x^m + C^{i\prime\prime} - (A_j' x^i + A_m' x^m \delta^i_j + B_j^i) V_{,j} \\ &+ 2(A_m' x^m + B') V_{,i} + V_{,ik}(A_m' x^m x^k + B_m^k x^m + C^k) \\ &+ V_{,it}(A_m x^m + B) = 0. \end{aligned} \tag{3.9}$$

Since the above symmetry formalism holds for n dimensions, we shall for generality now consider the dynamical equation (1.2) to also be n dimensional and take the potential energy V to be

$$V \equiv -\Phi(t)/r, \quad r^2 \equiv \delta_{ij} x^i x^j, \ i,j = 1,...,n. \tag{3.10}$$

With V so defined (3.8) may be expressed in the form

$$\Phi [A_k x^k \delta^i_m + 2A_m x^i] + r^3 [2A_m'' x^i + A_k'' x^k \delta^i_m + 2B_m^{i\prime} - B'' \delta^i_m] = 0. \tag{3.11}$$

Contraction of (3.11) on i and m gives

$$(n+2)\Phi [A_m x^m] + r^3 [(n+2) A_m'' x^m - nB'' + 2B_m^{m\prime}] = 0. \tag{3.12}$$

Note that the bracketed terms in (3.12) are polynomials in the x's. If we assume $n > 1$, the term r^3 is irrational in the

x's. Hence the bracketed terms must vanish, which implies

$$A_m = 0, \tag{3.13}$$

$$nB'' - 2B^{m\prime}_m = 0. \tag{3.14}$$

Use of (3.13) in (3.11) gives

$$B''\delta^i_m - 2B^{i\prime}_m = 0. \tag{3.15}$$

Note that (3.14) is a consequence of (3.15).

In (3.15), if $i \neq m$ we obtain

$$B^{i}_{m} = b^{i}_{m} = \text{consts}, \quad i \neq m. \tag{3.16}$$

In (3.15), if $i = m$ we have

$$B^{m\prime}_m = \tfrac{1}{2}B'', \quad m \text{ not summed}. \tag{3.17}$$

Hence

$$B^{1\prime}_1 = B^{2\prime}_2 = \cdots = B^{n\prime}_n = \tfrac{1}{2}B''. \tag{3.18}$$

Integration of (3.18) gives

$$B^i_i = \tfrac{1}{2}B' + b^i_i, \quad i \text{ not summed}, \ b^i_i = \text{consts}. \tag{3.19}$$

Equations (3.16) and (3.19) can be combined into the form

$$B^i_j = \tfrac{1}{2}B'\delta^i_j + b^i_j, \quad b^i_j = \text{consts}. \tag{3.20}$$

By inspection it is seen that (3.13) and (3.20) are necessary and sufficient for the solution of (3.11) when $n > 1$.

When $n = 1$, Eq. (3.11) reduces to

$$3\Phi A_1 + A_1''(x^1)^3 + [2B^{1\prime}_1 - B''](x^1)^2 = 0. \tag{3.21}$$

It is easily seen by inspection of (3.21) that (3.13) and (3.20) are also necessary and sufficient for solutions of (3.11) when $n = 1$.

By substitution of (3.10), (3.13), and (3.20) in (3.9), followed by multiplication by r^5, (3.9) may be expressed in the form

$$r^5[\tfrac{1}{2}B'''x^i + C^{i\prime\prime}] + x^i\{[(\Phi'B + \tfrac{1}{2}\Phi B')\delta^k_m - 3\Phi b^k_m]x^k x^m - 3\Phi C^k x^k\} = 0. \tag{3.22}$$

As in a similar situation above [refer to the statement following (3.12)] the bracketed terms in (3.22) must vanish individually if $n > 1$. Hence if $n > 1$

$$\tfrac{1}{2}B'''x^i + C^{i\prime\prime} = 0, \tag{3.23}$$

$$[(\Phi'B + \tfrac{1}{2}\Phi B')\delta^k_m - 3\Phi b^k_m]x^k x^m - 3\Phi C^k x^k = 0. \tag{3.24}$$

From (3.23) and (3.24) it follows that

$$B''' = 0, \tag{3.25}$$

$$C^k = 0, \tag{3.26}$$

$$(2\Phi'B + \Phi B')\delta^k_m - 3\Phi(b^k_m + b^m_k) = 0. \tag{3.27}$$

It follows from (3.27) that

$$b^k_m + b^m_k = 0, \quad k \neq m, \tag{3.28}$$

$$2\Phi'B + \Phi B' - 6\Phi b^m_m = 0, \quad m \text{ not summed}. \tag{3.29}$$

From (3.29) we obtain the conditions

$$\mu_1 \equiv b^1_1 = b^2_2 = \cdots = b^n_n = \frac{2\Phi'B + \Phi B'}{6\Phi}. \tag{3.30}$$

It is easily shown that (3.25), (3.26), (3.28), and (3.30) are necessary and sufficient for (3.22) to be satisfied when $n > 1$. It can be shown that these conditions are also necessary and sufficient when $n = 1$.

The constants b^i_j appearing in (3.28) and (3.30) may be expressed in the form

$$b^i_j = \omega^i_j + \mu_1\delta^i_j, \quad \omega^i_j = -\omega^j_i. \tag{3.31}$$

Use of (3.31) in (3.20) gives

$$B^i_j = (\tfrac{1}{2}B' + \mu_1)\delta^i_j + \omega^i_j. \tag{3.32}$$

By use of (3.13), (3.26), and (3.32) in (3.6), (3.7) we obtain the symmetry mapping functions ξ^i, ξ^0 in the form

$$\xi^i = (\tfrac{1}{2}B' + \mu_1)x^i + \omega^i_j x^j,$$

$$\omega^i_j (= -\omega^j_i), \ \mu_1 \text{ arbitrary const}, \tag{3.33}$$

$$\xi^0 = B, \tag{3.34}$$

where from (3.25) and (3.30)

$$B = \beta_2 t^2 + \beta_1 t + \beta_0,$$

$$\beta_0, \beta_1, \beta_2 = \text{arbitrary consts}, \tag{3.35}$$

and

$$2B\Phi' + \Phi B' = 6\mu_1\Phi. \tag{3.36}$$

If $B = 0$, then (3.36) shows that $\mu_1 = 0$, and hence (3.36) is satisfied identically. In this case $\Phi(t)$ is arbitrary and the symmetry functions ξ^i, ξ^0 of (3.33), (3.34) reduce to the familiar rotation

$$\xi^i = \omega^i_j x^j, \quad \xi^0 = 0. \tag{3.37}$$

This implies that every dynamical system (1.2) admits the rotation group, which of course is well known.

If $B \neq 0$, we may solve (3.36) for Φ in the form

$$\Phi(t) = \pm (k_1/B)^{-1/2} \exp\left(3\mu_1 \int B^{-1}\, dt\right), \tag{3.38}$$

with B given by (3.35).

Alternatively the solution of (3.36) for B in terms of Φ is given by

$$B = \Phi^{-2}\left[6\mu_1 \int \Phi^2\, dt + \mu_2\right], \quad \mu_2 \equiv \text{const}. \tag{3.39}$$

Note that (3.39) is valid for $B = 0$ as well as for $B \neq 0$. [If in (3.39) $B = 0$, then $\mu_1 = 0$ and $\mu_2 = 0$ and Φ will be arbitrary.]

It should be noted that the forms of $\Phi(t)$ corresponding to cases 1–3 in Sec. 2 are special cases of the form (3.38).

If a Noether mapping of the type (3.1), (3.2) exists for the dynamical system (1.2), then it will be a special case of the mapping defined by (3.33)–(3.36).[8] We shall now determine what additional restrictions the symmetry functions ξ^i, ξ^0 must satisfy in order to define a Noether symmetry mapping.

A Noether symmetry requires that there exist a function $\tau(x,t)$ such that the mapping (3.1), (3.2) satisfies

$$\delta\mathscr{L} + \mathscr{L}\frac{d}{dt}\delta t = -\frac{d\tau}{dt}\delta a, \tag{3.40}$$

where $\mathscr{L}$ is given by[9] (1.1) and $\delta\mathscr{L}$ is calculated by use of (3.1)–(3.3) and (3.5). By the expansion of (3.40) and the requirement that it hold identically in the $\dot{x}$'s we are led to the necessary and sufficient conditions

$$\xi^0_{,j} = 0, \tag{3.41}$$

$$\xi^i_{,j} + \xi^j_{,i} - \delta_{ij}\xi^0_{,t} = 0, \tag{3.42}$$

$$\xi^i_{,t} + \tau_{,i} = 0, \tag{3.43}$$

$$-\Phi x^i\xi^i + \Phi' r^2\xi^0 + \Phi r^2\xi^0_{,t} + r^3\tau_{,t} = 0. \tag{3.44}$$

By use of (3.33), (3.34) in (3.41)–(3.44) we obtain

$$2(\tfrac{1}{2}B' + \mu_1)\delta_{ij} - \delta_{ij}B' = 0, \tag{3.45}$$

$$\tfrac{1}{2}B''x^i + \tau_{,i} = 0, \tag{3.46}$$

$$-\Phi(\tfrac{1}{2}B' + \mu_1)r^2 + \Phi' r^2 B + \Phi r^2 B' + r^3\tau_{,t} = 0, \tag{3.47}$$

$$\mu_1 = 0, \tag{3.48}$$

$$\beta_2 x^i + \tau_{,i} = 0, \tag{3.49}$$

$$\Phi(\tfrac{1}{2}B' - \mu_1) + \Phi' B + r\tau_{,t} = 0. \tag{3.50}$$

From (3.49) we find

$$\tau = -\tfrac{1}{2}\beta_2 r^2 + f(t). \tag{3.51}$$

Use of (3.48) and (3.51) in (3.50) gives

$$\Phi B' + 2B\Phi' + 2rf' = 0. \tag{3.52}$$

It follows from (3.52) that $f = \beta_3 =$ arbitrary constant, which may be taken to be zero. Hence from (3.51)

$$\tau = -\tfrac{1}{2}\beta_2 r^2. \tag{3.53}$$

Use of (3.48) and (3.53) in (3.50) gives

$$2B\Phi' + \Phi B' = 0. \tag{3.54}$$

It follows from the above work that we may state the following theorem.

Theorem 3.1: A necessary and sufficient condition that n-dimensional dynamical equations of the form (1.2)′ (refer to Theorem 2.1) admit infinitesimal symmetry mappings of the form

$$\bar{x}^i = x^i + \delta x^i, \quad \delta x^i \equiv \xi^i(x,t)\delta a, \tag{3.1'}$$

$$\bar{t} = t + \delta t, \quad \delta t \equiv \xi^0(x,t)\delta a, \tag{3.2'}$$

is that

$$\xi^i = (\tfrac{1}{2}B' + \mu_1)x^i + \omega^i_j x^j,$$

$$\omega^i_j (= -\omega^j_i), \quad \mu_1 \text{ arbitrary consts,} \tag{3.33'}$$

$$\xi^0 = B, \tag{3.34'}$$

where

$$B \equiv \beta_2 t^2 + \beta_1 t + \beta_0, \quad \beta_0, \beta_1, \beta_2 \text{ arbitrary consts,} \tag{3.35'}$$

and the function $\Phi(t)$ appearing in the dynamical equations is determined by the condition

$$2B\Phi' + \Phi B' = 6\mu_1\Phi. \tag{3.36'}$$

This implies $\Phi(t)$ must be expressible in terms of the quadratic polynomial $B(t)$ by

$$\Phi(t) = \pm(k_1/B)^{-1/2}\exp\Big(3\mu_1\int B^{-1}\,dt\Big), \quad B \neq 0, \tag{3.38'}$$

or alternatively the quadratic polynomial B must satisfy

$$B = \Phi^{-2}\Big(6\mu_1\int\Phi^2\,dt + \mu_2\Big), \quad \mu_2 \text{ arbitrary const.} \tag{3.39'}$$

The functions ξ^i, ξ^0 given by (3.33)′, (3.34)′ will define Noether mappings in that they satisfy the condition

$$\delta\mathscr{L} + \mathscr{L}\frac{d}{dt}\delta t = -\frac{d\tau}{dt}\delta a, \tag{3.40'}$$

if and only if $\mu_1 = 0$ in (3.33) and

$$\tau = -\tfrac{1}{2}\beta_2 r^2. \tag{3.53'}$$

Corollary 3.1: If $B = 0$, $\Phi(t)$ is arbitrary and the corresponding (Noether) symmetry mappings admitted by the dynamical equations (1.2)′ are rotations.

For any Noether mapping (ξ^i, ξ^0, τ) it is well known[8] there will be a concomitant Noether constant of motion I_N given by the formula

$$I_N \equiv \frac{\partial\mathscr{L}}{\partial\dot{x}^i}\xi^i - \Big(\frac{\partial\mathscr{L}}{\partial\dot{x}^i}\dot{x}^i - \mathscr{L}\Big)\xi^0 + \tau. \tag{3.55}$$

In the next section it will be shown which of the constants of motion obtained in Sec. 2 are Noether constants of motion.

4. SYMMETRY GROUPS ADMITTED BY DYNAMICAL EQUATIONS (1.2) BASED ON Φ_1, Φ_2, AND Φ_3

In Sec. 2 we determined those $\Phi(t)$ (denoted by Φ_1, Φ_2, Φ_3) for which the corresponding dynamical equation (1.2) (considered to be of two or three dimensions) admitted first integrals of the form (1.3). In Sec. 3 we found the most general form of $\Phi(t)$ (3.38) such that the corresponding dynamical equations (1.2) [considered for generality to be n dimensional] would admit symmetry mappings of the form (3.1), (3.2). This general form for $\Phi(t)$ included (as mentioned in Sec. 3) the cases Φ_1, Φ_2, Φ_3 and restricted the mapping (3.1), (3.2) to be of the form (3.33), (3.34).

In this section we shall obtain the complete symmetry group admitted by each of the dynamical equations (1.2) (considered as n dimensional) determined, respectively, by Φ_2 and Φ_3. For each case we determine the Noether symmetry subgroup and obtain the concomitant Noether constants of motion. It is then shown that some of the constants of motion obtained in Sec. 2 are of the Noether form.

In the Appendix we give the remaining $\Phi(t)$, called Φ_4, Φ_5, Φ_6, for which the corresponding dynamical systems (1.2) admit symmetry mappings of the form (3.33), (3.34). Such dynamical systems will *not* admit quadratic first integrals (1.3) other than a quadratic function of the angular momentum.

It was noted in Sec. 3 [following (3.37)] that the rotation symmetry group was admitted by all dynamical systems (1.2) regardless of the form of $\Phi(t)$ [case 1, $\Phi_1(t) =$ arbitrary]. For all (nonconstant) $\Phi(t)$ except $\Phi_2(t)$, $\Phi_3(t)$, $\Phi_4(t)$, $\Phi_5(t)$, and $\Phi_6(t)$, the rotation group is the *complete* group of symmetries for the corresponding dynamical systems. Since for this rotation symmetry $\mu_1 = 0$ [refer to (3.33)–(3.37)], it follows from Theorem 3.1 that the rotation group is a Noether symmetry, and the concomitant Noether constants of motion (3.55) are angular momentum, as is well known.

There remain to be considered the symmetries of the dynamical systems defined when $\Phi(t)$ has the form Φ_2 or Φ_3.

We now consider case 2 for which $\Phi(t) = \Phi_2$ [refer to (2.64)]. By (3.39) and (2.64) we have

$$B = \frac{at^2 + bt + c}{\lambda_0^2}\Big[6\mu_1\int\frac{\lambda_0^2\,dt}{at^2 + bt + c} + \mu_2\Big]. \tag{4.1}$$

For the case $b^2-4ac<0$, (4.1) gives

$$B=\mu_2\left(\frac{at^2+bt+c}{\lambda_0^2}\right)+6\mu_1(at^2+bt+c)\times\left[\frac{2}{(4ac-b^2)^{1/2}}\arctan\left(\frac{2at+b}{(4ac-b^2)^{1/2}}\right)\right]. \quad (4.2)$$

A comparison of (4.2) and (3.35) shows that we must take $\mu_1=0$ and

$$\beta_2=\mu_2 a\lambda_0^{-2},\quad \beta_1=\mu_2 b\lambda_0^{-2},\quad \beta_0=\mu_2 c\lambda_0^{-2}. \quad (4.3)$$

Hence by (4.2) the mapping functions (3.33), (3.34) become

$$\xi^i=\tfrac{1}{2}\mu_2\left(\frac{2at+b}{\lambda_0^2}\right)x^i+\omega^i_j x^j, \quad (4.4)$$

$$\xi^0=\mu_2\left(\frac{at^2+bt+c}{\lambda_0^2}\right). \quad (4.5)$$

In (4.4) and (4.5) μ_2 and ω^i_j act as group parameters and lead to the symmetry mapping vectors

$$\xi^i(\mu_2)=\left(\frac{2at+b}{2\lambda_0^2}\right)x^i,$$

$$\xi^0(\mu_2)=\frac{at^2+bt+c}{\lambda_0^2}, \quad (4.6)$$

$$\xi^i(\omega^j_k)=\delta^i_k x^j-\delta^i_j x^k,\quad \xi^0(\omega^j_k)=0. \quad (4.7)$$

Based upon (4.6), (4.7) we obtain the generators

$$M_2\equiv\left(\frac{2at+b}{2\lambda_0^2}\right)x^i\partial_i+\left(\frac{at^2+bt+c}{\lambda_0^2}\right)\partial_t, \quad (4.8)$$

$$\Omega_{ij}\equiv x^i\partial_j-x^j\partial_i. \quad (4.9)$$

These generators define a $[1+n(n-1)/2]$-parameter group of symmetries.

For the case $b^2-4ac>0$ we find in a similar manner that again $\mu_1=0$ and we are led to the same generators (4.8), (4.9) and hence to the same symmetry group.

For any generator of the form

$$F\equiv f(t)x^i\partial_i+g(t)\partial_t,\quad f(t),g(t)\text{ arbitrary}, \quad (4.10)$$

it is easily shown that the commutator of F with any rotation generator Ω_{ij} vanishes identically, that is,

$$[F,\Omega_{ij}]\equiv 0. \quad (4.11)$$

Hence for the physically interesting case for which $n=3$, the dynamical equations with $\Phi=\Phi_2$ will admit the $G_4[M_2,\Omega_{ij}]$ with group algebra

$$[M_2,\Omega_{ij}]=0, \quad (4.12)$$

$$[\Omega_{12},\Omega_{23}]=-\Omega_{31},\quad [\Omega_{12},\Omega_{31}]=-\Omega_{23},$$
$$[\Omega_{23},\Omega_{31}]=-\Omega_{12}. \quad (4.13)$$

With reference to Theorem 3.1 (using general n) and the fact that $\mu_1=0$ in (4.4) and (4.5) it follows that the mappings defined by (4.6), (4.7) are Noether mappings.[10] From (3.53) and (4.3) we obtain for the mapping (4.6) the associated function

$$\tau(\mu_2)=-\frac{a}{2\lambda_0^2}r^2. \quad (4.14)$$

Use of (4.22) and (4.27) in (3.55) [with $\mathscr{L}$ of (1.1) generalized to n dimensions and based upon Φ_3 of (2.66)] leads to the Noether constant of motion

$$I_N(\mu_2)=-\frac{1}{\lambda_0^2}\left\{(at^2+bt+c)\left[\tfrac{1}{2}\delta_{ij}\dot{x}^i\dot{x}^j-\frac{\lambda_0}{r(at^2+bt+c)^{1/2}}\right]-\tfrac{1}{2}(2at+b)\delta_{ij}x^i\dot{x}^j+\frac{a}{2}r^2\right\}. \quad (4.15)$$

Comparison of E_2 (2.74) with $I_N(\mu_2)$ of (4.15) with $n=2$ shows

$$E_2=-\lambda_0^2 I_N(\mu_2). \quad (4.16)$$

We now obtain the symmetry group of the dynamical equation (1.2) for the case in which $\Phi(t)=\Phi_3$ [refer to (2.66)]. Again for generality we assume general n.

From (3.39) and (2.66) we find

$$B=-\frac{6\mu_1(\alpha t+\beta)}{\alpha}+\mu_2\left(\frac{\alpha t+\beta}{\lambda_0}\right)^2. \quad (4.17)$$

Comparison of (4.17) and (3.35) shows that

$$\beta_2=\mu_2\frac{\alpha^2}{\lambda_0^2},\quad \beta_1=\frac{2\mu_2\alpha\beta}{\lambda_0^2}-6\mu_1,$$

$$\beta_0=\frac{\mu_2\beta^2}{\lambda_0^2}-\frac{6\mu_1\beta}{\alpha}. \quad (4.18)$$

By use of (4.17) in (3.33) and (3.34) we obtain

$$\xi^i=\mu_1(-2x^i)+\mu_2\times\left(\frac{\alpha}{\lambda_0^2}(\alpha t+\beta)\right)x^i+\omega^i_j x^j, \quad (4.19)$$

$$\xi^0=\mu_1\left(-\frac{6}{\alpha}(\alpha t+\beta)\right)+\mu_2\left(\frac{\alpha t+\beta}{\lambda_0}\right)^2, \quad (4.20)$$

where μ_1, μ_2, and ω^i_j are the $2+n(n-1)/2$ parameters of the symmetry group. Hence we obtain $2+n(n-1)/2$ symmetry mapping vectors given by (4.7) and

$$\xi^i(\mu_1)=-2x^i,\quad \xi^0(\mu_1)=-\frac{6}{\alpha}(\alpha t+\beta), \quad (4.21)$$

$$\xi^i(\mu_2)=\frac{\alpha}{\lambda_0^2}(\alpha t+\beta)x^i,$$

$$\xi^0(\mu_2)=\left(\frac{\alpha t+\beta}{\lambda_0}\right)^2. \quad (4.22)$$

The above symmetry vectors lead to the generators (4.9) and

$$\bar{M}_1\equiv-2x^i\partial_i-\frac{6}{\alpha}(\alpha t+\beta)\partial_t, \quad (4.23)$$

$$\bar{M}_2\equiv\frac{\alpha}{\lambda_0^2}(\alpha t+\beta)x^i\partial_i+\left(\frac{\alpha t+\beta}{\lambda_0}\right)^2\partial_t. \quad (4.24)$$

These generators define the symmetry group of the n-dimensional generalization of the dynamical equation (1.2) for the case $\Phi=\Phi_3$. When $n=3$, the commutators of this group are given by (4.13) and

$$[\bar{M}_1,\bar{M}_2]=-6\bar{M}_2, \quad (4.25)$$

$$[\bar{M}_\gamma,\Omega_{ij}]=0,\quad \gamma=1,2. \quad (4.26)$$

[Equation (4.26) follows from (4.10), (4.11).]

With reference to Theorem 3.1 (general n) the mapping based on $\bar{M}_2$ [see (4.22) and (4.24)] is a Noether symmetry. From (3.53) and (4.18) the associated function $\tau(\mu_2)$ for this mapping is

$$\tau(\mu_2) = -\tfrac{1}{2}(\alpha/\lambda_0)^2 r^2. \tag{4.27}$$

Use of (4.22) and (4.27) in (3.55) [with $\mathscr{L}$ of (1.1) generalized to n dimensions and based upon Φ_3 of (2.66)] leads to the Noether constant of motion

$$I^*_N(\mu_2) = -\frac{1}{\lambda_0^2}\Big\{(\alpha t+\beta)^2\Big[\tfrac{1}{2}\delta_{ij}\dot{x}^i\dot{x}^j - \frac{\lambda_0}{r(\alpha t+\beta)}\Big] - \alpha(\alpha t+\beta)\delta_{ij}x^i\dot{x}^j + \tfrac{1}{2}\alpha^2 r^2\Big\}. \tag{4.28}$$

Comparison of E_3 (2.80) with $I^*_N(\mu_2)$ of (4.28) with $n=2$ shows

$$E_3 = -\lambda_0^2 I^*_N(\mu_2). \tag{4.29}$$

The results of this section are summarized in the theorem to follow.

Theorem 4.1: With reference to Theorems 2.1 and 3.1: (a) When $\Phi = \Phi_2$ or Φ_3 the corresponding n-dimensional dynamical equation of the form (1.2) admits the Noether symmetry (in addition to rotations) defined by

$$\xi^i(\mu_2) = \frac{x^i}{2}\frac{d}{dt}(\Phi^{-2}),\quad \xi^0(\mu_2) = \Phi^{-2},$$
$$\tau(\mu_2) = -\frac{r^2}{4}\frac{d^2}{dt^2}(\Phi^{-2}). \tag{4.30}$$

(b) When $\Phi = \Phi_3$ the corresponding n-dimensional dynamical equation of the form (1.2) admits in addition to the Noether symmetries mentioned in (a) the non-Noether symmetry

$$\xi^i(\mu_1) = -2x^i,\quad \xi^0(\mu_1) = -\frac{6}{\alpha}(\alpha t+\beta). \tag{4.21$'$}$$

(c) When $\Phi = \Phi_2$ the Noether symmetries mentioned in (a) form a group of $[1 + n(n-1)/2]$ parameters defined by the generators

$$\Omega_{ij} \equiv x^i\partial_j - x^j\partial_i, \tag{4.9$'$}$$
$$M_2 \equiv \Big(\frac{2at+b}{2\lambda_0^2}\Big)x^i\partial_i + \Big(\frac{at^2+bt+c}{\lambda_0^2}\Big)\partial_t. \tag{4.8$'$}$$

In case $n=3$ the group algebra is given by

$$[M_2,\Omega_{ij}] = 0, \tag{4.12$'$}$$
$$[\Omega_{12},\Omega_{23}] = -\Omega_{31},\quad [\Omega_{12},\Omega_{31}] = -\Omega_{23},$$
$$[\Omega_{23},\Omega_{31}] = -\Omega_{12}. \tag{4.13$'$}$$

(d) When $\Phi = \Phi_3$ the symmetries mentioned in (a) and (b) above form a group of $[2 + (n-1)/2]$ parameters defined by the generators (4.9)$'$ and

$$\bar{M}_1 \equiv -2x^i\partial_i - \frac{6}{\alpha}(\alpha t+\beta)\partial_t, \tag{4.23$'$}$$
$$\bar{M}_2 \equiv \frac{\alpha}{\lambda_0^2}(\alpha t+\beta)x^i\partial_i + \Big(\frac{\alpha t+\beta}{\lambda_0}\Big)^2\partial_t. \tag{4.24$'$}$$

In case $n=3$ the group algebra is given by (4.13)$'$ and

$$[\bar{M}_1,\bar{M}_2] = -6\bar{M}_2, \tag{4.25$'$}$$
$$[\bar{M}_\gamma,\Omega_{ij}] = 0,\quad \gamma = 1,2. \tag{4.26$'$}$$

(e) When $\Phi = \Phi_2$ or Φ_3 the Noether constant of motion [of the n-dimensional dynamical equation of the form (1.2)]

$$I_N \equiv \frac{\partial\mathscr{L}}{\partial\dot{x}^i}\xi^i(\mu_2) - \Big(\frac{\partial\mathscr{L}}{\partial\dot{x}^i}\dot{x}^i - \mathscr{L}\Big)\xi^0(\mu_2) + \tau(\mu_2) \tag{3.55$'$}$$

concomitant with the Noether symmetry (4.30) mentioned in (a) is found to be

$$I_N = \lambda_0^{-2}E, \tag{4.31}$$

where E is given by (2.86). [Refer to Theorem 2.1 (d) and Corollary (2.1).]

5. ORBIT EQUATIONS FOR THE DYNAMICAL SYSTEM WITH $\Phi(t) = \Phi_3$

We shall now determine the orbit equations for the two-dimensional dynamical system (1.2) for case 3 for which $\Phi(t) = \Phi_3$ of (2.66). This will be done by use of the two constants of motion A_1 and A_2 [refer to (2.78), (2.79)] which are the components of the vector constant of motion (2.83).

Based upon the above-mentioned Φ_3 the dynamical equations (1.2) in plane-polar coordinates (r,ϕ) take the form

$$\ddot{r} - r\dot{\phi}^2 = \frac{\lambda_0}{(\alpha t+\beta)r^2}, \tag{5.1}$$
$$r\ddot{\phi} + 2\dot{r}\dot{\phi} = 0. \tag{5.2}$$

Equation (5.2) leads immediately to the angular momentum constant of motion

$$L = r^2\dot{\phi} \doteq l_0,\quad l_0 = \text{const}. \tag{5.3}$$

In the r,ϕ coordinates the two constants of motion A_1 and A_2 referred to above may be expressed in the respective forms

$$l_0(\psi\dot{r} - \mu_0 r)\sin\phi - (1 - l_0\psi r\dot{\phi})\cos\phi \doteq k_x, \tag{5.4}$$
$$-l_0(\psi\dot{r} - \mu_0 r)\cos\phi - (1 - l_0\psi r\dot{\phi})\sin\phi \doteq k_y, \tag{5.5}$$

where

$$\psi \equiv (\alpha t+\beta)/\lambda_0 = \Phi_3^{-1},\quad \mu_0 \equiv \alpha/\lambda_0. \tag{5.6}$$

If (5.4) and (5.5) are solved for the coefficients of the $\sin\phi$ and $\cos\phi$ terms and (5.3) is used to eliminate $\dot{\phi}$, then the resulting equations lead immediately to

$$l_0^2\psi/r = S, \tag{5.7}$$
$$\psi\dot{r} - \mu_0 r = -S'/l_0, \tag{5.8}$$

where

$$S = S(\phi) \equiv 1 + k_x\cos\phi + k_y\sin\phi, \tag{5.9}$$
$$S' = -k_x\sin\phi + k_y\cos\phi, \tag{5.10}$$

and where the prime denotes differentiation with respect to ϕ.

By use of (5.7) we eliminate ψ from (5.8) to obtain

$$r\dot{r}S + l_0S' = \mu_0 l_0^2 r. \tag{5.11}$$

We now transform (5.1) and (5.11) to u,ϕ variables [where it is assumed $u = u(\phi)$] by means of the relation

$$u = 1/r \tag{5.12}$$

and (5.3) to obtain, respectively,

$$u'' + u = u/S, \tag{5.13}$$

$$u'S - S'u = -\mu_0 l_0. \tag{5.14}$$

We note that the function $u'S - S'u$ of (5.14) is a first integral of the (dynamical) equation (5.13).

From (5.14) we obtain

$$(u/S)' = -\mu_0 l_0/S^2, \tag{5.15}$$

which upon integration gives

$$u = S\left[-\mu_0 l_0 \int \frac{d\phi}{S^2} + c_0\right], \quad c_0 = \text{const.} \tag{5.16}$$

By use of (5.6), (5.9), and (5.12) we may express (5.16) in terms of the r,ϕ variables to obtain the orbit equations of the dynamical system (5.1) in the form

$$\frac{1}{r} = (1 + k_x \cos\phi + k_y \sin\phi) \times\left[-l_0 \frac{\alpha}{\lambda_0} \int \frac{d\phi}{(1 + k_x \cos\phi + k_y \sin\phi)^2} + c_0\right]. \tag{5.17}$$

The orbit equation (5.17) can be rewritten in the form

$$\frac{1}{r} = c_0[1 + e\cos(\phi - \gamma)] - \frac{\alpha l_0}{\lambda_0}[1 + e\cos(\phi - \gamma)] \times \int \frac{d\phi}{[1 + e\cos(\phi - \gamma)]^2}, \tag{5.18}$$

where e and γ are defined by

$$k_x = e\cos\gamma, \quad k_y = e\sin\gamma, \tag{5.19}$$

and

$$e^2 = k_x^2 + k_y^2. \tag{5.20}$$

With reference to (2.85) we note that

$$e^2 = 1 + 2l_0^2 k^*/\lambda_0^2. \tag{5.21}$$

If we reduce the dynamical equation to the usual time-independent Kepler problem by choosing $\alpha = 0$ so that $\Phi = \Phi_3$ reduces to a constant [refer to (2.66)], then the orbit equation (5.18) reduces to the familiar equation of a conic[3]

$$1/r = c_0[1 + e\cos(\phi - \gamma)], \tag{5.22}$$

in which case e given by (5.20) defines the eccentricity.

With Φ_3 reduced to a constant, Eq. (5.21) can be interpreted as the usual relationship between eccentricity e and the value of angular momentum l_0 and energy k^* associated with the dynamical curve (5.22).[11] [Refer to (2.80) and the last paragraph of Sec. 2.] However for the *time-dependent* Φ_3 we must regard (5.21) as a generalized formula where l_0 is still the value of the angular momentum but where k^* and e are now analogous, respectively, to the energy and eccentricity.

For the case of *time-independent* Φ the value of the eccentricity ($e > 1, e = 1, e < 1, e = 0$) determines the nature of the conic orbit. In a similar manner the value of the constant e determines the nature of the more general orbits given by (5.18) for the *time-dependent* Φ_3 case. For the *time-dependent* Φ_3 we shall now consider the orbit equation (5.18) for each of the above-mentioned e's.

A. The case $e = 0$

For the case $e = 0$ we note from (5.20) that $k_x = k_y = 0$, and from (5.21) that $k^* = -\lambda_0^2/2l_0^2$.

With $e = 0$ the orbit equation (5.18) leads to

$$r = \frac{1}{c_0 - (\alpha l_0/\lambda_0)\phi}, \tag{5.23}$$

which is recognized as a spiral. As α tends to zero (or equivalently as Φ_3 approaches a constant value) the spiral orbit (5.23) approaches in the limit the circular orbit $r = 1/c_0$ associated with the time-independent case $\alpha = 0$.

For this $e = 0$ case r and ϕ are easily expressible as functions of t. Since $e = 0$ implies $k_x = k_y = 0$, we obtain by means of (5.6)–(5.9)

$$r(t) = l_0^2(\alpha t + \beta)/\lambda_0. \tag{5.24}$$

If $r = r_0$ when $t = t_0$ we obtain from (5.24)

$$r(t) = r_0\left(\frac{\alpha t + \beta}{\alpha t_0 + \beta}\right). \tag{5.25}$$

If (5.23) is evaluated at $t = t_0$ [$\phi(t_0) \equiv \phi_0$] we obtain

$$c_0 = \frac{1}{r_0} + \frac{\alpha l_0}{\lambda_0}\phi_0. \tag{5.26}$$

Use of (5.25), (5.26), and (5.3) evaluated at t_0 in (5.23) gives [$(d\phi/dt)_0 \equiv \dot{\phi}_0$]

$$\phi(t) = \phi_0 + \frac{\lambda_0(t - t_0)}{r_0^3 \dot{\phi}_0(\alpha t + \beta)}. \tag{5.27}$$

B. The case $e = 1$

For the case $e = 1$ we note from (5.20) that

$$k_x^2 + k_y^2 = 1, \tag{5.28}$$

and from (5.21) we find $k^* = 0$. With $e = 1$, the orbit equation (5.18) takes the form

$$\frac{1}{r} = c_0[1 + \cos(\phi - \gamma)] - \frac{\alpha l_0}{\lambda_0}[1 + \cos(\phi - \gamma)] \times \int \frac{d\phi}{[1 + \cos(\phi - \gamma)]^2}. \tag{5.29}$$

Upon carrying out the integration in (5.29) the result can be written in the form

$$\frac{1}{r} = c_0[1 + \cos(\phi - \gamma)] - \frac{\alpha l_0}{3\lambda_0} \times \left[\frac{\sin(\phi - \gamma)[2 + \cos(\phi - \gamma)]}{1 + \cos(\phi - \gamma)}\right]. \tag{5.30}$$

We note that as α tends to zero (or equivalently as Φ_3 approaches a constant value) the orbit (5.30) approaches a parabola.

As an illustration of the nature of the orbit for the case $e = 1$, (5.30), we find for the choice $c_0 = 0$ and $\alpha l_0/(3\lambda_0) = -1$ that the orbit equation in rectangular coordinates has the form

$$x^2 = \frac{y(2y-1)^2}{2-3y}, \tag{5.31}$$

which is recognized as a form of a strophoid.[12,13]

C. The case $e < 1$

For the case $e<1$ we note from (5.22) that

$$k_x^2 + k_y^2 < 1, \tag{5.32}$$

and from (5.23) that $k^* < 1$.

Evaluation of the integral in (5.20) for the case $e<1$ allows us to express the orbit equation in the form

$$\frac{1}{r} = c_0[1 + e\cos(\phi-\gamma)] - \frac{\alpha l_0[1+e(\phi-\gamma)]}{\lambda_0(1-e^2)^{3/2}} \times\left[\arccos\left(\frac{e+\cos(\phi-\gamma)}{1+e\cos(\phi-\gamma)}\right) - \frac{e(1-e^2)^{1/2}\sin(\phi-\gamma)}{1+e\cos(\phi-\gamma)}\right]. \tag{5.33}$$

As α approaches zero the orbit approaches an ellipse.

D. The case $e > 1$

For the case $e>1$ we note from (5.22) that

$$k_x^2 + k_y^2 > 1 \tag{5.34}$$

and from (5.23) that $k^* > 1$.

Upon integration of the integral in (5.20) for case $e>1$ we may express the orbit equation in the form

$$\frac{1}{r} = c_0[1+e\cos(\phi-\gamma)] - \frac{\alpha l_0}{\lambda_0}\frac{[1+e\cos(\phi-\gamma)]}{(e^2-1)^{3/2}} \times\left\{\frac{e(e^2-1)^{1/2}\sin(\phi-\gamma)}{1+e\cos(\phi-\gamma)} - \ln\left[\frac{e+\cos(\phi-\gamma)+(e^2-1)^{1/2}\sin(\phi-\gamma)}{1+e\cos(\phi-\gamma)}\right]\right\}. \tag{5.35}$$

As α tends to zero the orbit approaches a hyperbola.

APPENDIX

Complete groups of symmetries for n-dimensional dynamical systems of the form (1.2) based upon Φ_4, Φ_5, or Φ_6, respectively, are given. These groups will contain in addition to the rotation group one non-Noether symmetry. However, when $n=3$ the corresponding three-dimensional dynamical systems (1.2) will not admit quadratic first integrals other than quadratic functions of the angular momentum.

We list below each of the above-mentioned Φ's, and concomitant ξ^i, ξ^0 that define the generators of the complete group of symmetries.

Case Φ_4:

$$\Phi_4(t) \equiv \frac{\lambda_0}{t-\gamma}\exp\left(\frac{\nu}{t-\gamma}\right), \quad \lambda_0,\nu,\gamma = \text{const}, \quad \nu\neq 0. \tag{A1}$$

$$\xi^i(\mu_1) = \left[1 - \frac{3}{\nu}(t-\gamma)\right]x^i, \qquad \xi^0(\mu_1) = -\frac{3}{\nu}(t-\gamma)^2, \tag{A2}$$

$$\xi^i(\omega^j_k) = \delta^i_k x^j - \delta^i_j x^k, \quad \xi^0(\omega^j_k) = 0. \tag{A3}$$

The generators of the complete group are given by

$$M_4 \equiv \left[1 - \frac{3}{\nu}(t-\gamma)\right]x^i\partial_i - \frac{3}{\nu}(t-\gamma)^2\partial_t, \tag{A4}$$

$$\Omega_{ij} \equiv x^i\partial_j = x^j\partial_i. \tag{A5}$$

These generators define a $[1+n(n-1)/2]$-parameter group, which for $n=3$ has the group algebra [refer to (4.11)]

$$[M_4,\Omega_{ij}] = 0, \tag{A6}$$

$$[\Omega_{12},\Omega_{23}] = -\Omega_{31}, \quad [\Omega_{12},\Omega_{31}] = -\Omega_{23}, \quad [\Omega_{23},\Omega_{31}] = -\Omega_{12}. \tag{A7}$$

Case Φ_5:

$$\Phi_5(t) \equiv \lambda_0(t-\gamma)^{\nu-1/2}(t-\delta)^{-\nu-1/2}, \quad \lambda_0,\gamma,\delta = \text{const}, \quad \gamma\neq\delta, \quad \nu\neq 0. \tag{A8}$$

$$\xi^i(\mu_1) = \left[1 + \frac{3(2t-\gamma-\delta)}{2\nu(\gamma-\delta)}\right]x^i, \qquad \xi^0(\mu_1) = \frac{3(t-\gamma)(t-\delta)}{\nu(\gamma-\delta)}, \tag{A9}$$

$$\xi^i(\omega^j_k) = \delta^i_k x^j - \delta^i_j x^k, \quad \xi^0(\omega^j_k) = 0. \tag{A10}$$

The generators of the complete group are given by (A5) and

$$M_5 \equiv \left[1 + \frac{3(2t-\gamma-\delta)}{2\nu(\gamma-\delta)}\right]x^i\partial_i + \frac{3(t-\gamma)(t-\delta)}{\nu(\gamma-\delta)}\partial_t. \tag{A11}$$

These generators define a $[1+n(n-1)/2]$-parameter group, which for $n=3$ has the group algebra defined by (A7) and

$$[M_5,\Omega_{ij}] = 0. \tag{A12}$$

Case Φ_6:

$$\Phi_6(t) \equiv \lambda_0[(t-\gamma)^2+\delta^2]^{-1/2} \times \exp\left[\frac{\nu}{\delta}\arctan\left(\frac{t-\gamma}{\delta}\right)\right], \quad \lambda_0,\gamma,\delta,\nu = \text{const}, \quad \nu\neq 0, \quad \delta\neq 0. \tag{A13}$$

$$\xi^i(\mu_1) = [1 + (3/\nu)(t-\gamma)]x^i, \qquad \xi^0(\mu_1) = (3/\nu)[(t-\gamma)^2+\delta^2], \tag{A14}$$

$$\xi^i(\omega^j_k) \equiv \delta^i_k x^j - \delta^i_j x^k, \quad \xi^0(\omega^j_k) = 0. \tag{A15}$$

The generators of the complete group are given by (A5) and

$$M_6 \equiv [1 + (3/\nu)(t-\gamma)]x^i\partial_i + (3/\nu)[(t-\gamma)^2+\delta^2]\partial_t. \tag{A16}$$

These generators define a $[1+n(n-1)/2]$-parameter group, which for $n=3$ has the group algebra defined by (A7) and

$$[M_6,\Omega_{ij}] = 0. \tag{A17}$$

[1]The coordinates x^i will denote rectangular coordinates in Euclidean space. Repeated indices satisfy the Einstein summation convention. A dot over a symbol indicates total time derivative. A comma (,) indicates partial differ-

entiation. A primed symbol (′) denotes differentiation with respect to the indicated argument.

[2]For references to the time-varying G problem refer to the survey article by P. S. Wesson, Physics Today **33**, 32 (July, 1980).

[3]H. Goldstein, *Classical Mechanics*, 2nd ed. (Addison-Wesley, Reading, MA, 1980).

[4]The symbol ($\doteq$) denotes equality on a dynamical path, that is for those $x^i = x^i(t)$ that are solutions of the dynamical equations (1.2).

[5]In the analysis of case 3 we assumed $\alpha \neq 0$ to exclude the time-independent case.

[6]It is well known that, by use of what is generally referred to as the inverse Noether theory, corresponding to any constant of motion there will exist a concomitant *velocity-dependent* Noether mapping. However, such mappings in general will not be unique and they may or may not be symmetry mappings of the dynamical equation, that is, they may not map the solution set of the dynamical equation into itself. For references to the inverse Noether theory see for example W. Sarlet and F. Cantrijn, "Generalization of Noether's Theorem in Classical Mechanics," to appear in SIAM Rev. (1981).

[7]G. H. Katzin and J. Levine, J. Math Phys. **18**, 1267 (1977).

[8]G. H. Katzin and J. Levine, J. Math Phys. **17**, 1345 (1976). Refer to Theorem 3.2 of this reference.

[9]We are continuing with the assumption that the system is n dimensional and hence r^2 in (1.1) is understood to be n dimensional.

[10]Equation (4.7) defines rotations, and therefore will not be treated in detail. It is well known that the associated $\tau(\omega^j_k) = 0$ and the concomitant Noether constant of motion is angular momentum.

[11]Refer to Eq. (3.57) of Ref. 3.

[12]G. James and R. James, *Mathematical Dictionary* (*Multilingual Edition*) (Van Nostrand, New York, 1959).

[13]We acknowledge the computational assistance of L. R. Katzin for plotting the strophoid curve.

Direct and inverse scattering problems of the nonlinear intermediate long wave equation

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The inverse scattering transformation method associated with a nonlinear singular integrodifferential equation is discussed. The equation describes long internal gravity waves in a stratified fluid of finite depth, and reduces to the Korteweg–de Vries equation as shallow water limit and the Benjamin–Ono equation as deep water limit. Both limits of the method and novel aspects of the theory are also discussed.

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1. INTRODUCTION

In recent years, there has been considerable physical and mathematical interest in a certain nonlinear singular integrodifferential equation,[1–6]

$$u_t + (1/\delta)u_x + 2uu_x + Tu_{xx} = 0, \tag{1.1}$$

where $T(\cdot)$ is the singular integral operator given by

$$(Tf)(x) = \frac{1}{2\delta} P\int_{-\infty}^{\infty} \coth \frac{\pi(y-x)}{2\delta} f(y)\, dy \tag{1.2}$$

($P\int_{-\infty}^{\infty}$ represents the principal value integral). Physically, Eq. (1.1) describes the long internal gravity waves in a stratified fluid with finite depth (characterized by the parameter δ). Depending on the parameter δ, (1.1) reduces to the Korteweg–de Vries (KdV) equation as $\delta \to 0$ (shallow-water limit),

$$u_t + 2uu_x + (\delta/3)u_{xxx} = 0, \tag{1.3}$$

and the Benjamin–Ono (BO) equation as $\delta \to \infty$ (deep-water limit),

$$u_t + 2uu_x + Hu_{xx} = 0. \tag{1.4}$$

Here $H(\cdot)$ is the Hilbert transform given by

$$(Hf)(x) = \frac{1}{\pi} P\int_{-\infty}^{\infty} \frac{1}{y-x} f(y)\, dy. \tag{1.5}$$

Hence Eq. (1.1) is an intermediary equation between those two very interesting nonlinear evolution equations, (describing certain long wave motion). It is now known that (1.1) has an N-soliton solution,[3,4] infinite number of conservation lows, a Bäcklund transformation and a novel type of inverse scattering transform (IST) to solve the initial value problem.[6,7]

In this paper, we discuss in detail the direct and inverse problems of this new scattering problem. This paper serves to amplify and extend the results of our previous note.[7] In Sec. 2, we reformulate the IST scheme, originated in Ref. 6, with a specific analytical requirement in the complex x plane, say z plane. Specifically, the scattering problem may be viewed as a differential Riemann–Hilbert problem. In Sec. 3, we discuss the direct scattering problem, and define specific Jost functions in terms of a Green function. Then we show that the Jost function satisfies a Fredholm type integral equation. This is unlike the usual situations where we have local scattering problems (e.g., Schrödinger equation) and where the Jost function satisfies the Volterra integral equation. Several remarkable features of the Green function corresponding to the limits $\delta \to 0$, $\delta \to \infty$ are discussed in Appendix A. Using the results obtained in the previous sections, Sec. 4 is devoted to solving the inverse problem within a certain class of initial conditions. For this class of initial conditions we construct the linear integral equation (i.e., a Gel'fand–Levitan type equation) and hence give the direct connection between the solution of (1.1) and the scattering data defined in Sec. 3. In Sec. 5, using the Gel'fand–Levitan equation, we obtain an explicit form of the N-soliton solution, and in Sec. 6, taking the analyticity of the scattering data into account, we give the trace formula for the scattering function, and we express the conserved quanitities in terms of the scattering data. In Secs. 4–6 we keep δ finite in order for use to be sure of the appropriate analyticity of our Jost functions. We discuss the case $\delta = \infty$ (the BO limit) in Sec. 7, and we illustrate several remarkable properties of the scattering problem in this case. Our basic philosophy regarding the BO equation is to obtain the information by taking the limit process $\delta \to \infty$. However, we are careful to point out that we do not present here the solution to the initial value problem of the BO equation. Nevertheless we feel that the analysis presented here should be a basis for extension to the BO equation.

2. IST SCHEME

The IST Scheme[6] for (1.1) is given by

$$i\psi_x^+ + (u-\lambda)\psi^+ = \mu\psi^-, \tag{2.1}$$

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$$i\psi_t^\pm + 2i(\lambda + 1/2\delta)\psi_x^\pm + \psi_{xx}^\pm + [\mp iu_x - Tu_x + \nu]\psi^\pm = 0, \tag{2.2}$$

where λ and μ are constants given by $\lambda = -k\coth 2k\delta$, $\mu = k\,\mathrm{cosech}\, 2k\delta$, and ν is a constant determined by fixing the Jost functions of (2.1) (see Sec. 3). Here $\psi^\pm(x)$ represent the boundary values of functions $\left[\text{i.e., } \psi^\pm(x) = \lim_{\mathrm{Im}\, z\to 0} \psi^\pm(z)\right]$ analytic in the horizontal strips between $\mathrm{Im}\, z = 0$ and $\mathrm{Im}\, z = \pm 2\delta$, and periodically extended vertically. By using the operator $T(\cdot)$, $\psi^\pm(x)$ may be written in the form

$$\psi^+(x) = \lim_{\mathrm{Im}\, z\downarrow 0} \psi(z) = \tfrac{1}{2}(1 - iT)\Psi(x), \tag{2.3a}$$

$$\psi^-(x) = \lim_{\mathrm{Im}\, z\uparrow 0} \psi(z) = -\tfrac{1}{2}(1 + iT)\Psi(x), \tag{2.3b}$$

where $\Psi(x)$ defined on the real axis is a proper fuction for the operator $T(\cdot)$ (i.e., $|\int_{-\infty}^{\infty}\Psi(x)\,dx| < \infty$, and $\Psi(x)$ satisfies the Hölder condition on the real axis, i.e., there exists constants C and h such that $|\Psi(x) - \Psi(y)| < C|x-y|^h, 0 < h \leqslant 1$), and for $\mathrm{Im}\, z \neq 0 (\mathrm{mod}\ 2\delta)$, $\psi(z)$ is given by

$$\psi(z) = \frac{1}{4\delta i}\int_{-\infty}^{\infty} \coth\frac{\pi(y-z)}{2\delta}\,\Psi(y)\,dy. \tag{2.4}$$

From (2.3) and (2.4), we have a relation

$$T(\psi^+ - \psi^-) = i(\psi^+ + \psi^-). \tag{2.5}$$

It should be noted that the relation (2.5) due to the analyticity requirement is weaker than condition (27) in Ref. 6 in a sense (i.e., if $\ln\psi^+$ is analytic, then so is ψ^+). Furthermore, from the periodicity (period 4δ) of (2.4), we have the relation between $\psi^\pm(x)$ in the form of difference

$$\psi^-(x) = \psi^+(x + 2i\delta). \tag{2.6}$$

We also note that the same constant can be added to $\psi^\pm(x)$ without violating the analytically requirement. With regard to the limits $\delta\to 0$ and $\delta\to\infty$, we make some remarks.

Remark 1: As mentioned in Ref. 6, for $\delta\to 0$, the scattering problem (2.1) tends to the Schrödinger equation with $\phi(x) = \lim_{\delta\to 0}\psi^\pm(x)$, i.e.,

$$\delta(\phi_{xx} + k^2\phi) + u\phi = 0, \tag{2.7}$$

and for $\delta\to\infty$,

$$i\psi_x^+ + (u + k)\psi^+ = 2k\psi^-, \quad \text{for } k > 0, \tag{2.8}$$

where $\psi^\pm(z)$ are the functions analytic in the upper and lower half z plane.

Remark 2: The formula (2.4) with the limit $\delta\to\infty$ is just the Plemelj formula, that is, as $\delta\to\infty$, $\frac{1}{2}(1 \mp iT)(\cdot)$ in (2.3) tend to the usual projection operators $P^\pm(\cdot) = \frac{1}{2}(1 \mp iH)(\cdot)$ that decompose a function into two functions analytic in the upper and lower half z plane.

3. DIRECT SCATTERING PROBLEM

Here and in Secs. 4–6 we assume for convenience that the initial condition $u(x,0)$ decays sufficiently rapidly as $|x|\to\infty$. In order to analyze the direct scattering problem of (2.1), it is convenient to define a new function,

$$W(x;k) \equiv \psi(x;k)\exp(ikx), \tag{3.1}$$

where we have defined $\psi(x;k) \equiv \psi^\pm(x \pm i\delta;k)$ and $W(x;k) \equiv W^\pm(x \pm i\delta;k)$ by taking (2.6) into account. Hereafter, for functions $f^\pm(x)$, we shall frequently use the notion $f(x)$ in which $f^\pm(x) = f(x \mp i\delta)$.

From (3.1) Eqs. (2.1) and (2.2) become

$$iW_x^+ + (\zeta_+ + 1/2\delta)(W^+ - W^-) = -uW^+, \tag{3.2}$$

$$iW_t^\pm - 2i\zeta_+ W_x^\pm + W_{xx}^\pm + [\mp iu_x - Tu_x + \rho]W^\pm = 0, \tag{3.3}$$

where $\rho = -2k\zeta_+ + k^2 + \nu$, $\zeta_\pm = \zeta_\pm(k) = k \pm (k\coth 2k\delta - 1/2\delta)$ (we shall need the definition of ζ_- subsequently). The solution to (3.2) can be given by an integral equation,

$$W(x;k) = W_0(x;k) + \int_{-\infty}^{\infty} G(x,y;k)u(y)W^+(y;k)\,dy, \tag{3.4}$$

where $W_0(x;k)$ is the solution of the homogeneous equation of (3.2) [i.e., $u(x) = 0$], and $G(x,y;k)$ is a Green function satisfying

$$i\frac{\partial}{\partial x}G^+(x,y;k) + (\zeta_+ + 1/2\delta)[G^+(x,y;k) - G^-(x,y;k)] = -\delta(x-y). \tag{3.5}$$

Here $G^\pm(x,y;k) = G(x \mp i\delta\sigma, y;k)$. From (3.5), we have the Fourier representation of the Green function $G(x,y;k)$,

$$G(x,y;k) = \frac{1}{2\pi}\int_C dp\,\hat{G}(p;k)e^{ip(x-y)} \tag{3.6}$$

in which $\tilde{G}(p;k)$ are given by

$$\hat{G}(p;k) = \left[pe^{p\delta} - 2k\frac{\sinh p\delta}{\sinh 2k\delta}e^{2k\delta}\right]^{-1} = \frac{p}{2}\,\mathrm{cosech}(p\delta)\left\{p\left[\zeta_+\left(\frac{p}{2}\right) - \zeta_+(k)\right]\right\}^{-1}, \tag{3.7}$$

where the contour C is taken to be a contour (from $-\infty$ to ∞) determined by choosing the specific solution to (3.2) (see below). In Appendix A, we discuss the properties of the Green function in both limits $\delta\to 0$ and $\delta\to\infty$. From (3.7), we see that $\hat{G}(p;k)$ have poles at $p = 0$, $p = 2\zeta_+^{-1}[\zeta_+(k)]$. Since $\zeta_+^{-1}(\cdot)$ is the multivalued function, we have an infinite number of poles for which we shall define $p_{-1} = 0$, $p_0 = 2k$ and $p_n, \bar{p}_n$ $(n \geqslant 1)$ such that, for $n \geqslant 1$, $(2n-1)\pi/(2\delta) < \mathrm{Im}\, p_n < (2n+3)\pi/(2\delta)$ and similarly for $-\mathrm{Im}\,\bar{p}_n$. Moreover double zero poles occur at special values of $\zeta_+(k)$ satisfying $\zeta_+(k) = 0$ and $p_n = \zeta_+(k)$, $\bar{p}_n = \zeta_+(k)$ $(n \geqslant 1)$ [i.e., $p_n = p_{n-1}, \bar{p}_n = \bar{p}_{n-1} (n \geqslant 0)$]. We call these values $\zeta_+^{(0)} = 0$ and $\{\zeta_+^{(i)}, \bar{\zeta}_+^{(i)}\}_{i=1}^\infty (\mathrm{Im}\,\zeta_+^{(i)} > 0, \mathrm{Im}\,\bar{\zeta}_+^{(i)} < 0)$. Considering the equations of p_n $(n \geqslant 0)$,

$$\frac{dp_n}{d\zeta_+} = \frac{p_n}{2\delta(p_n - \zeta_+)(\zeta_+ + 1/2\delta)} \tag{3.8}$$

($\bar{p}_n$ satisfy same equation), one can see that there are logarithmic branch points at $\zeta_+ = -1/2\delta$ for p_0, p_n and $\bar{p}_n$ $(n \geqslant 1)$, and square root branch points at $\{\zeta_+^{(1)}, \bar{\zeta}_+^{(1)}\}$ for p_0, at

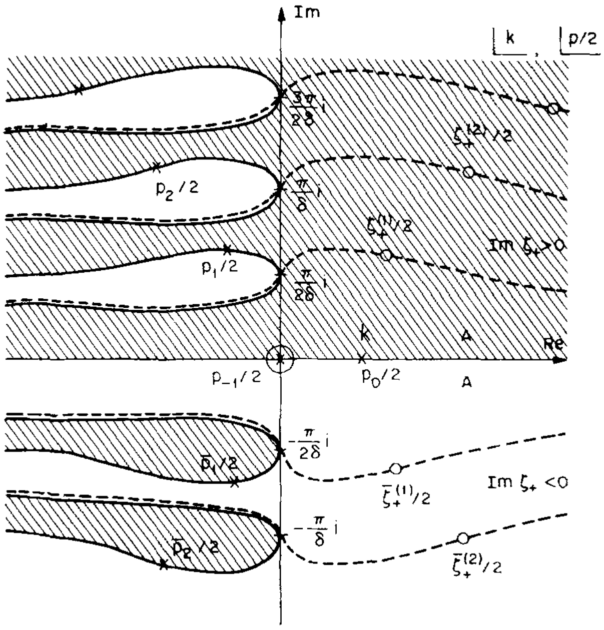

FIG. 1. The k plane (or $p/2$ plane). For given k, $\times$ and O denote the poles $p_{-1}=0, p_0, \{p_i, \bar{p}_i\}_{i=1}^{\infty}$, and the double poles $\zeta_+^{(0)}=0, \{\zeta_+^{(i)}, \bar{\zeta}_+^{(i)}\}_{i=1}^{\infty}$ of Eq. (3.7), respectively. Each branch is surrounded by the dotted line, and branch A is the principal branch (PB). The shaded regions correspond to the upper half ζ_+ plane (multisheeted).

$\{\zeta_+^{(n)}, \zeta_+^{(n+1)}\}$ for p_n, and at $\{\bar{\zeta}_+^{(n)}, \bar{\zeta}_+^{(n+1)}\}$ for $\bar{p}_n$, respectively. It should be noted that from the multiplicity of k $(=\zeta_+^{-1}(\cdot))$, we are required to define an appropriate branch in k plane. We show in Fig. 1 the several of the branches in k plane, and in Fig. 2 the fundamental sheet (abbreviated hereafter as FS) corresponding to the principal branch (as PB), which is the portion A including the real k axis in Fig. 1.

From (3.2), one can see that if $W(x;k)$ is a solution, then $W(x;-k)\exp(2ikx)$ is also a solution. Taking this into account we now define specific Jost functions of (3.2). For real k, the Jost functions are defined as the solution to (3.2) with the boundary conditions

$$\left.\begin{array}{l} M(x;k)\to 1, \\ \bar{M}(x;k)\to e^{2ikx}, \end{array}\right\} \quad \text{as } x\to -\infty, \tag{3.9a,b}$$

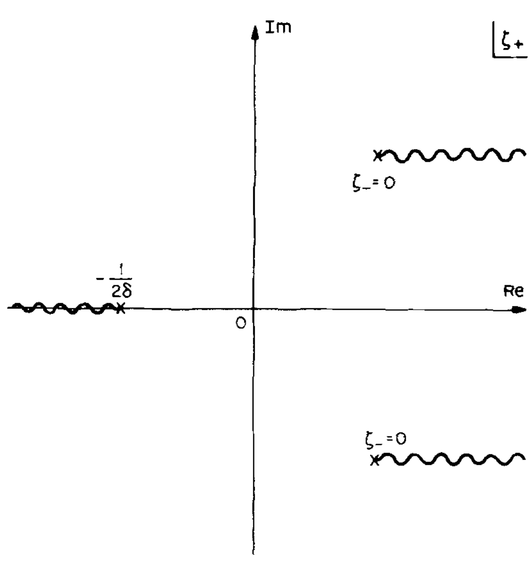

FIG. 2. The fundamental sheet (FS) corresponding to the principal branch. The wave lines show the branch cuts corresponding to the edges of PB.

$$\left.\begin{array}{l} N(x;k)\to e^{2ikx}, \\ \bar{N}(x;k)\to 1, \end{array}\right\} \quad \text{as } x\to \infty. \tag{3.10a,b}$$

Here note that $\bar{M}(x;k)=M(x;-k)\exp(2ikx)$ and $\bar{N}(x;k)=N(x;-k)\exp(2ikx)$. Then in terms of the Green function (3.6), these Jost functions are given by

$$\begin{pmatrix} M(x;k) \\ \bar{M}(x;k) \end{pmatrix} = \begin{pmatrix} 1 \\ e^{2ikx} \end{pmatrix} = \int_{-\infty}^{\infty} G_1(x,y;k)u(y) \begin{pmatrix} M^+(y;k) \\ \bar{M}^+(y;k) \end{pmatrix} dy, \tag{3.11a,b}$$

$$\begin{pmatrix} N(x;k) \\ \bar{N}(x;k) \end{pmatrix} = \begin{pmatrix} e^{2ikx} \\ 1 \end{pmatrix} + \int_{-\infty}^{\infty} G_2(x,y;k)u(y) \begin{pmatrix} N^+(y;k) \\ \bar{N}^+(y;k) \end{pmatrix} dy, \tag{3.12a,b}$$

where the contours $C_{1,2}$ for $G_{1,2}(x,y;k)$ are taken to be the lines $\mathrm{Re}\,(p-i0)$, $\mathrm{Re}(p+i0)$, respectively [this is necessary in order to preserve the boundary conditions (3.9) and (3.10)]. Note that by taking these contours the Green functions $G_{1,2}(x,y;k)$ are bounded as $|x|\to\infty$. It is important to remark that (3.11) and (3.12) are Fredholm type integral equations, unlike the usual case of the local scattering problem (e.g., Schrödinger equation) where the Jost functions satisfy the Volterra type integral equations. In addition, we note that by using residue calculus (3.11) and (3.12) can be represented in an explicit manner useful for the proof of existence and analyticity of the solution (see Appendix B). As shown in Appendix B, we have the following propositions:

(i) $M(x;k)$, $\bar{N}(x;k)$ have convergent Neumann series in certain region of the FS for given δ and $\max|u|$ chosen small enough.

(ii) Despite the fact mentioned below Eq. (3.8) (i.e., the poles have square root branch points in the FS), $M(x;k)$ and $\bar{N}(x;k)$ are holomorphic in the upper and lower half plane of the FS, respectively. Moreover they are analytic in these regions, whenever the Neumann series converges in this region. In addition, we have the asymptotic form of $M(x;k)$ and $\bar{N}(x;k)$,

$$M(x;k)\to 1+O\left(\frac{1}{\zeta_1}\right) \text{ as } |\zeta_+|\to\infty, \quad \mathrm{Im}\,\zeta_+>0, \tag{3.13}$$

$$\bar{N}(x;k)\to 1+O\left(\frac{1}{\zeta_1}\right) \text{ as } |\zeta_+|\to\infty, \quad \mathrm{Im}\,\zeta_+<0. \tag{3.14}$$

We now define the appropriate scattering data corresponding to the Jost functions (3.11) and (3.12). For real k [i.e., $\zeta_+ > -1/(2\delta)$], by virtue of the fact that

$$G_1(x,y;k) - G_2(x,y;k)$$
$$= \frac{1}{2i\delta\zeta_+} - \frac{1}{2i\delta\zeta_-}\exp[2ik(x-y)-2k\delta], \tag{3.15}$$

we have alternative representations for $M(x;k)$ and $N(x;k)$, respectively,

$$M(x;k) = a(k) + b(k)e^{2ikx} + \int_{-\infty}^{\infty} G_2(x,y;k)u(y)M^+(y;k)\,dy, \tag{3.16}$$

$$N(x;k) = \bar{a}(k)e^{2ikx} + \bar{b}(k) + \int_{-\infty}^{\infty} G_1(x,y;k)u(y)N^+(y;k)\,dy. \tag{3.17}$$

Here $a(k)$, $b(k)$, $\bar{a}(k)$ and $\bar{b}(k)$ are given by

$$a(k) = 1 + \frac{1}{2i\delta\zeta_+}\int_{-\infty}^{\infty} dy\, u(y)M^+(y;k), \tag{3.18a}$$

$$b(k) = -\frac{1}{2i\delta\zeta_-}\int_{-\infty}^{\infty} dy\, u(y)M^+(y;k)e^{-2ik(y-i\delta)}, \tag{3.18b}$$

$$\bar{a}(k) = 1 + \frac{1}{2i\delta\zeta_-}\int_{-\infty}^{\infty} dy\, u(y)N^+(y;k)e^{-2ik(y-i\delta)}, \tag{3.19a}$$

$$\bar{b}(k) = \frac{1}{2i\delta\zeta_+}\int_{-\infty}^{\infty} dy\, u(y)N^+(y;k). \tag{3.19b}$$

When the solutions of the integral equations (3.16) and (3.17) are unique (or having a convergent Neumann series as a stronger condition), then we have

$$M(x;k) = a(k)\bar{N}(x;k) + b(k)N(x;k) \tag{3.20}$$

and

$$N(x;k) = \bar{a}(k)\bar{M}(x;k) + \bar{b}(k)M(x;k), \tag{3.21}$$

which are considered as "right" and "left" scattering equations, respectively. Moreover, as shown in Appendix C, one finds

$$\bar{a}(k) = a^*(-k), \tag{3.22a}$$

$$\bar{b}(k) = -b(-k) = -\left(\frac{d\zeta_+}{dk}\right)\left(\frac{d\zeta_-}{dk}\right)^{-1} b^*(k), \tag{3.22b}$$

$$|a(k)|^2 - \left(\frac{d\zeta_+}{dk}\right)\left(\frac{d\zeta_-}{dk}\right)^{-1}|b(k)|^2 = 1. \tag{3.23}$$

From (3.18a), we note that $a(k)$ takes on the same analyticity as $M(x;k)$, and $a(k)\to 1$ as $|\zeta_+|\to\infty$, $\operatorname{Im}\zeta_+\geqslant 0$.

On the other hand, for $\zeta_+ + i0$ with $\zeta_+ < -1/(2\delta)$ and ζ_+ real [i.e., k is in the upper half plane at the edge of the *PB* where $\zeta_+(k) = \zeta_+ = \zeta_+(k^*)$] we have a relation

$$G_1(x,y;k) - G_2(x,y;k^*) = \frac{1}{2i\delta\zeta_+}, \tag{3.24}$$

from which we have

$$M(x;k) = a(k) + \int_{-\infty}^{\infty} G_2(x,y;k^*)u(y)M^+(y;k)\,dy, \tag{3.25}$$

$$\bar{N}(x;k^*) = \bar{a}(-k^*) + \int_{-\infty}^{\infty} G_1(x,y;k)u(y)\bar{N}^+(y;k^*)\,dy. \tag{3.26}$$

Here we have used the relation $\bar{N}(x;k) = N(x;-k)\exp(2ikx)$. From (3.25) and (3.26), we obtain

$$M(x;k) = a(k)\bar{N}(x;k^*), \tag{3.27}$$

$$\bar{N}(x;k^*) = \bar{a}(-k^*)M(x;k) \tag{3.28}$$

[i.e., $a(k)\bar{a}(-k^*) = 1$], whenever the solutions of (3.25) and (3.26) are unique.

The bound states defined as

$$M(x;k)\to 0 \quad \text{as} \quad x\to+\infty \tag{3.29}$$

and

$$N(x;k)\to 0 \quad \text{as} \quad x\to-\infty \tag{3.30}$$

are given by

$$a(k_l) = 0, \quad M(x;k_l) = b_l N(x;k_l) \tag{3.31}$$

and

$$\bar{a}(\bar{k}_l) = 0, \quad N(x;\bar{k}_l) = \bar{b}_l M(x;\bar{k}_l), \tag{3.32}$$

with $\bar{k}_l = -k_l^*$ for $l = 1,2,\ldots,N$. As shown in Appendix D, $a(k)$ has only simple zeroes and they lie on the imaginary k axis, i.e., $k_l = i\kappa_l = \bar{k}_l$, $0<\kappa_l<\pi/2\delta$ in the PB, and $b_l\bar{b}_l = 1$. The right and left scattering datas are now given by

$$S_R = [a(k), b(k), \{\kappa_l, b_l\}_{l=1}^N], \tag{3.33}$$

$$S_L = [\bar{a}(k), \bar{b}(k), \{\kappa_l, \bar{b}_l\}_{l=1}^N]. \tag{3.34}$$

Let us now find the time evolution of the scattering data. By virtue of the boundary condition (3.9), the constant ρ in (3.3) is taken to be zero. From (3.3), (3.20), and (3.27), we obtain

$$a(k,t) = (k,0), \tag{3.35a}$$

$$b(k,t) = b(k,0)\exp[-4ik(\lambda + 1/2\delta)t], \tag{3.35b}$$

$$b_l(t) = b_l(0)\exp[4\kappa_l(\lambda_l + 1/2\delta)t], \tag{3.35c}$$

where $\lambda_l = \lambda(i\kappa_l) = -\kappa_l\cot 2\kappa_l\delta$.

Before closing this section, we offer several remarks:

Remark 1: Although there are infinitely many solutions to (3.2) corresponding to the poles of (3.7), we have chosen only a finite set of solutions as the Jost functions where the Green functions are bounded as $|x|\to\infty$ for real k, that is, (3.9) and (3.10). As shown in Appendix E, however, when we have a unique solution to the integral equation (3.4) [e.g., in the case that the Neumann series of the integral equation (3.4) converges], our set of the Jost functions (3.11) [or (3.12)] consists of a complete set of the functions in the sense of $L_2(-\infty<x<\infty)$.

Remark 2: In order to define the scattering data (3.33) [or (3.34)], we have assumed that the solution of the integral equation (3.4) is unique (and we have given sufficient conditions on δ, $\max|u|$ for this to hold), mathematically speaking, there is to be no nontrivial solution of the homogeneous equation of (3.4), i.e.,

$$W_h^+(x;k) = \int_{-\infty}^{\infty} G^+(x,y;k)u(y)W_h^+(y;k)\,dy. \tag{3.36}$$

However, in general, the solutions $W_h^+(x;k)$ may exist for some k [certainly for $\delta\to\infty$ (see Sec. 7) we refer to such values of k as "eigenvalues" of the Fredholm integral equation]. In this case, the solution to (3.4) may have a singularity, unless $W_0^+(x;k)$ satisfies

$$\int_{-\infty}^{\infty}[W_h^A(x;k)W_0(x;k)]^+\,dx = 0,$$

where $W_h^A(x;k)$ is the solution of the adjoint equation of (3.36),

$$[W_h^A(x;k)]^+ = u(x)\int_{-\infty}^{\infty} G^+(y,x;k)[W_h^A(y;k)]^+\,dy,$$

and we must add this eigenvalue into the scattering data (it may be a new kind of bound state). We shall discuss briefly such situations in Sec. 7.

4. INVERSE SCATTERING PROBLEM

We now discuss the inverse scattering problem associated with (3.2) in the case when the integral equations for the Jost functions have a unique solution and the Jost functions are analytic in certain region of the FS.

For $\bar{N}(x;k)$, from the analyticity and the asymptotic behavior (3.14), the following integral representation is suggested:

$$\bar{N}(x;k) = 1 + \int_x^\infty ds\, K(x,s) e^{i\zeta_+(x-s)} \quad \text{for } \operatorname{Im}\zeta_+ < 0. \tag{4.1}$$

Substituting (4.1) into (3.2) and (3.3), one finds that the kernel $K(x,y)$ satisfies

$$\{i\partial_x + 1/2\delta + u(x)\}K^+(x,y) + (i\partial_y - 1/2\delta)K^-(x,y) = 0, \tag{4.2}$$

$$\{i\partial_t + \partial_x^2 - \partial_y^2 + 2(\partial_x K(x,x))\}K(x,y) = 0, \tag{4.3}$$

with

$$u(x) = iK^+(x,x) - iK^-(x,x), \tag{4.4}$$

where $K^\pm(x,y) = K(x \mp i\delta, y \mp i\delta)$ and $K(x,y) \to 0$ as $y \to \infty$. It is important to note that (4.4) is a decomposition of $u(x)$ (see Sec. 2), and from (2.5) we also have the relation,

$$(Tu)(x) = -\{K^+(x,x) + K^-(x,x)\}. \tag{4.5}$$

Subject to (4.4) and (4.5), one can see that the compatibility between (4.2) and (4.3) gives Eq. (1.1).

From (4.1) and the relation $N(x;k) = \bar{N}(x;-k)\exp(2ikx)$, we also have

$$N(x;k) = e^{2ikx}\left[1 + \int_x^\infty ds\, K(x,s) e^{-i\zeta_-(x-s)}\right], \tag{4.6}$$

which is analytic in the upper half ζ_- plane [note $\zeta_+(-k) = -\zeta_-(k)$]. By virtue of the triangular representations (4.1) and (4.6) one can derive the linear integral equation (i.e., a Gel'fand–Levitan type equation) and hence solve the inverse problem as follows: dividing (3.20) and (3.27) by $a(k)$ and operating with $(1/2\pi)\int_{-\infty}^{\infty} d\zeta_+ \exp[i\zeta_+(y-x)]$. (i.e., Fourier transform) for $y > x$, we have

$$\begin{aligned}\frac{1}{2\pi}\int_{-\infty+i0}^{\infty+i0} d\zeta_+ \frac{M(x;k)}{a(k)} e^{i\zeta_+(y-x)} &= \frac{1}{2\pi}\int_{-\infty-i0}^{\infty-i0} d\zeta\, \bar{N}(x;k) e^{i\zeta_+(y-x)} \\ &\quad + \frac{1}{2\pi}\int_{-1/2\delta}^{\infty} d\zeta_+ \frac{b(k)}{a(k)} N(x;k) e^{i\zeta_+(y-x)}.\end{aligned} \tag{4.7}$$

From the analyticity arguments for $M(x;k)$ and $a(k)$ (i.e., analytic on the upper half plane of the FS), the left-hand side of (4.7) can be written in the form

$$-\sum_{l=1}^N C_l N(x; i\kappa_l) \exp[i\zeta_{+l}(y-x)], \tag{4.8}$$

where $C_l = -ib_l/\dot{a}_l$, $\dot{a}_l = \partial a/\partial\zeta_+|_{\zeta_+=\zeta_{+l}}$, $\zeta_{+l} = \zeta_+(i\kappa_l)$. Then, using (4.1) and (4.6), we obtain the Gel'fand–Levitan equation,

$$K(x,y) + F(x,y) = \int_x^\infty K(x,s) F(s,y)\, ds = 0 \quad \text{for } y > x, \tag{4.9}$$

with

$$F(x,y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk \left(\frac{d\zeta_+}{dk}\right)\frac{b(k)}{a(k)} e^{i\zeta_- x + i\zeta_+ y} + \sum_{l=1}^N C_l \exp(i\zeta_{-l}x + i\zeta_{+l}y), \tag{4.10}$$

(note $\int_{-\infty}^{\infty} dk\,(d\zeta_+/dk)\cdot = \int_{-1/2\delta}^{\infty} d\zeta_+\cdot$). In Sec. 5, by using (4.9), we construct the N-soliton solution as an example of an explicit solution of (1.1).

To close this section, we briefly discuss an alternative method of the inverse problem which is a direct method[8] based upon the Gel'fand–Levitan equation (4.9). From (4.10), taking $(\zeta_+ + 1/2\delta) = (-\zeta_- + 1/2\delta)\exp(4k\delta)$ into account, one finds that $F(x,y)$ satisfies

$$(i\partial_x + 1/2\delta)F^+(x,y) + (i\partial_y - 1/2\delta)F^-(x,y) = 0. \tag{4.11}$$

From (3.35), we also have

$$(i\partial_t + \partial_x^2 - \partial_y^2)F(x,y) = 0. \tag{4.12}$$

From (4.9), (4.11), and (4.12) one can derive (4.2) and (4.3) with (4.4) whose compatibility yields (1.1) with (4.5). Then the direct method based upon (4.9) is given as follows: For given $u(x,0)$,

(1) find $K^\pm(x,y,0)$ from (4.2) with the boundary condition $K^\pm(x,x,0) = \mp iu^\pm(x,0)$ $[u(x,0) = u^+(x,0) + u^-(x,0)$ from (4.4)],

(2) find $F^\pm(x,y,0)$ from (4.9),

(3) find $F^\pm(x,y,t)$ from (4.12),

(4) find $K^\pm(x,y,t)$ from (4.9),

(5) then $u(x,t) = iK^+(x,x,t) - iK^-(x,x,t)$.

5. N-SOLITON SOLUTION

In the case of an N-soliton solution, $F(x,y)$ in the Gel'fand–Levitan equation is given by

$$F(x,y) = \sum_{l=1}^N C_l \exp(i\zeta_{-l}x + i\zeta_{+l}y), \tag{5.1}$$

where C_l is a positive real function of t (see Appendix D). In order to solve (4.9) with (5.1), we assume $K(x,y)$ to be of the form

$$K(x\, y) = \sum_{l=1}^N (C_l)^{1/2}\Gamma_l(x)\exp(i\zeta_{+l}y). \tag{5.2}$$

Then (4.9) becomes

$$\Gamma_n + i\sum_{l=1}^N \frac{(C_n C_l)^{1/2} e^{i(\zeta_{-n}+\zeta_{+l})x}}{\zeta_{-n}+\zeta_{+l}}\Gamma_l = -C_n^{1/2} e^{i\zeta_{-n}x}. \tag{5.3}$$

Here we note that the matrix $\Delta(x)$ defined by

$$[\Delta(x)]_{nl} = i(C_n C_l)^{1/2}\frac{\exp[i(\zeta_{-n}+\zeta_{+l})x]}{\zeta_{-n}+\zeta_{+l}} \tag{5.4}$$

is positive definite. Namely, for an arbitrary column vector $\mathbf{V} = (v_1,\ldots,v_N)^T$ the inner product $(\mathbf{V},\Delta\,\mathbf{V}) \equiv (\mathbf{V}^T)^*\Delta\,\mathbf{V}$ takes positive value, i.e., noting $(\zeta_{+l})^* = -\zeta_{-l}$,

$$(\mathbf{V},\Delta\,\mathbf{V}) = i\sum_{n,l} v_n^* \frac{(C_n C_l)^{1/2} e^{i(\zeta_{-n}+\zeta_{+l})x}}{\zeta_{-n}+\zeta_{+l}} v_l$$
$$= \int_x^\infty \left|\sum_n^N C_n^{1/2} v_n \exp(i\zeta_{+n} s)\right|^2 ds > 0. \tag{5.5}$$

Therefore, for $\mathbf{\Gamma} \equiv (\Gamma_l,\ldots,\Gamma_N)^T$, we have

$$\mathbf{\Gamma} = (I+\Delta)^{-1}\mathbf{E} \tag{5.6}$$

where $\mathbf{E} \equiv (E_l,\ldots,E_N)^T$ with the element $E_l = -C_l^{1/2}\exp(i\zeta_{-l}x)$. From (5.6), we obtain

$$K(x,x) = \frac{\partial}{\partial x}\ln\det|I+\Delta(x)|, \tag{5.7}$$

which leads to

$$u(x,t) = i\frac{\partial}{\partial x}\ln\det\left|\frac{I+\Delta(x-i\delta,t)}{I+\Delta(x+i\delta,t)}\right|, \tag{5.8}$$

where I is the identity matrix. For example, a 1-soliton solution is given by

$$u(x,t) = \frac{2\kappa_1\sin(2\kappa_1\delta)}{\cos(2\kappa_1\delta)+\cosh\{2\kappa_1[x-x_1(t)]\}}, \tag{5.9}$$

where κ_1 is an eigenvalue, $k = i\kappa_1$, and from (3.35) $x_l(t)$ is given by

$$x_1(t) = \frac{1}{2\kappa_1}\ln\frac{C_1(t)}{2\kappa_1}$$
$$= (2\lambda_1+\delta^{-1})t + x_1(0). \tag{5.10}$$

For N-soliton solution, following the method developed in Ref. 9, one can calculate the phase shift formula for l th-soliton,

$$x_l^+(0) - x_l^-(0)$$
$$= \frac{1}{\kappa_l}\ln\left[\sum_{m=l+1}^{N}\left|\frac{\zeta_{+l}+\zeta_{-m}}{\zeta_{+l}-\zeta_{+m}}\right|\sum_{m=1}^{l-1}\left|\frac{\zeta_{+m}-\zeta_{+l}}{\zeta_{-m}+\zeta_{+l}}\right|\right]. \tag{5.11}$$

Here we have ordered $\kappa_l > \kappa_2 > \cdots > \kappa_N > 0$, and $x_l^\pm(0)$ are the phases of the soliton at $t\to\pm\infty$, respectively.

It is interesting to note that the N-soliton solution (5.8) can be written in terms of the squared eigenfunctions. From (5.3) we have

$$C_l N_l = -C_l^{1/2}\Gamma_l\exp(i\zeta_{+l}x) \tag{5.12}$$

and

$$N_n = e^{-2\kappa_n x}\left[1 - i\sum_{l=1}^{N}\frac{C_l N_l}{\zeta_{-n}+\zeta_{+l}}\right], \tag{5.13}$$

where $N_l(x) = N(x;i\kappa_l)$. Then we obtain

$$u(x) = iK^+(x,x) - K^-(x,x)$$
$$= -i\sum_{l=1}^{N} C_l[N_l^+(x) - N_l^-(x)]$$
$$= 2\sum_{l=1}^{N} C_l\sin(2\kappa_l\delta)|N_l^+|^2 e^{2\kappa_l x}. \tag{5.14}$$

On the other hand, from (2.1) or (3.2), one finds that the equation for $\Psi \equiv |\psi^+|^2 = |W^+\exp[-ik(x-i\delta)]|^2$ with k real or pure imaginary satisfies

$$\psi_t + (1/\delta)\Psi_x + 2u\Psi_x + T\Psi_{xx} = 0, \tag{5.15}$$

which is the associated linear equation of (1.1). Note that this result is similar to the case of the KdV equation.[9] In fact, the results obtained in Ref. 9 for the KdV solitons are derived by taking $\lim \delta\to 0$ in our results.

6. CONSERVATION LAWS

As shown in Ref. 6, (1.1) has an infinite number of conservation laws. Here we give the direct connection between those conserved quantities and the scattering data defined in the Sec. 3. We first show that the function defined by

$$\sigma(x;k) = \ln\frac{M^-(x;k)}{M^+(x;k)} \tag{6.1}$$

is directly related to the scattering data $a(k)$. Noting that, for large ζ_+ in the upper half plane of the FS, $M^\pm(x;k)$ are not zero, we have a relation

$$(T\sigma)(x;k) = -i\ln[M^+(x;k)M^-(x;k)A], \tag{6.2}$$

for large $|\zeta_+|$, Im $\zeta_+ > 0$, where we have used the fact mentioned below Eq. (2.6), and the constant A can be determined by the boundary condition (see below). It should be noted that $\sigma(x)\to 0$ as $|x|\to\infty$, since for Im $\zeta_+ > 0$ in the FS, $M^\pm(x;k)\to 1$ as $x\to-\infty$ and $M^\pm(x;k)\to a(k)$ as $x\to+\infty$. From (6.1) and (6.2), (4.2) and (4.3) become

$$e^\sigma - 1 = \frac{1}{2\zeta_+}\left[\frac{1}{\delta}(1-e^\sigma) - i\sigma_x - T\sigma_x + 2u\right], \tag{6.3}$$
$$\sigma_t - 2\zeta_+\sigma_x - i\sigma_{xx} + \sigma_x T\sigma_x + 2u_x = 0. \tag{6.4}$$

Taking $\int_{-\infty}^{\infty}\sigma_x T\sigma_x\,dx = 0$ into account, from (6.4), one finds that $\sigma(x)$ is a conserved density. For large $|\zeta_+|$, (6.3) has an asymptotic expansion

$$\sigma(x;k) = \sum_{n=1}^{\infty}\frac{\phi_n(x)}{(2\zeta_+)^n}. \tag{6.5}$$

The first two $\phi_n(x)$ are

$$\phi_1 = 2u,$$
$$\phi_2 = -2u^2 - \frac{2}{\delta}u - 2iu_x - 2T(u_x). \tag{6.6}$$

On the other hand, from the definition of $T(\cdot)$, we have

$$(T\sigma)(x;k) \to \begin{cases} -\dfrac{1}{2\delta}\displaystyle\int_{-\infty}^{\infty}\sigma(y;k)\,dy & \text{as } x\to\infty, \\ \dfrac{1}{2\delta}\displaystyle\int_{-\infty}^{\infty}\sigma(y;k)\,dy & \text{as } x\to-\infty, \end{cases} \tag{6.7}$$

and from the boundary conditions of $M^\pm(x;k)$ for Im $\zeta_+ > 0$,

$$\ln[M^+(x;k)M^-(x;k)A] \to \begin{cases}\ln[a^2(k)\mathrm{A}] & \text{as } x\to+\infty, \\ \ln A & \text{as } x\to-\infty.\end{cases} \tag{6.8}$$

Comparing (6.7) with (6.8), we obtain

$$\ln a(k) = -\frac{i}{2\delta}\int_{-\infty}^{\infty}\sigma(y;k)\,dy. \tag{6.9}$$

Next we derive a closed form expression for $a(k)$ by using the analyticity requirements of the previous sections.

Namely, we employ the following facts:

(i) $a(k)$ is analytic for $\mathrm{Im}\,\zeta_+ > 0$.

(ii) $a(k)$ has only a finite number of simple zeros.

(iii) $a(k) \to 1$, as $|\zeta_+| \to \infty$ for $\mathrm{Im}\,\zeta_+ \geqslant 0$.

(iv) $a(k) = \bar{a}^*(-k^*)$ for real $\zeta_+(k)$.

In this case, $a(k)$ can be written in the form

$$a(k) = \hat{a}(k) \prod_{l=1}^{N} \frac{\zeta_+ - \zeta_{+l}}{\zeta_+ + \zeta_{-l}}, \tag{6.10}$$

where, for $\mathrm{Im}\,\zeta_+ \geqslant 0$, $\hat{a}(k)$ has no zeros and $\hat{a}(k) \to 1$ as $|\zeta_+| \to \infty$. From (6.10) we obtain

$$a(k) = \left(\prod_{l=1}^{N} \frac{\zeta_+ - \zeta_{+l}}{\zeta_+ + \zeta_{-l}} \right) \times \exp\left[\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\zeta'_+}{\zeta'_+ - \zeta_+} \ln|a[k'(\zeta'_+)]|^2 \right],$$

for $\mathrm{Im}\zeta_+ > 0$, (6.11)

$$a(k) = \lim_{\mathrm{Im}\,\zeta_+ \downarrow 0} a(k), \quad \text{for real } \zeta_+.$$

For large $|\zeta_+|$, we have the asymptotic expansion,

$$\ln a(k) = \frac{1}{2\delta} \sum_{n=1}^{\infty} \frac{1}{(2\zeta_+)^n} \left[\frac{2^n}{\pi} \int_{-\infty}^{\infty} (\zeta'_+)^{n-1} \ln|a(k')|^2 \, d\zeta'_+ + \frac{2^{n+1}\delta i}{n} \sum_{l=1}^{N} \{\zeta^n_{+l} - \zeta^{*n}_{+l}\} \right]. \tag{6.12}$$

Comparing (6.5) with (6.12), we now obtain the trace formula

$$I_n \equiv \int_{-\infty}^{\infty} \phi_n(y)\, dy = -\frac{2^n\delta}{\pi} \int_{-\infty}^{\infty} d\zeta_+ \, \zeta_+^{n-1} \ln|a(k)|^2 - \frac{2^{n+1}}{n} i\delta \sum_{l=1}^{N} \{\zeta^n_{+l} - \zeta^{*n}_{+l}\}. \tag{6.13}$$

From the first two terms of I_n, we have

$$\int_{-\infty}^{\infty} u\, dx = 4 \sum_{l=1}^{N} \kappa_l \delta - \frac{\delta}{\pi} \int_{-\infty}^{\infty} d\zeta_+ \ln|a(k)|^2, \tag{6.14a}$$

$$\int_{-\infty}^{\infty} u^2\, dx = 8 \sum_{l=1}^{N} \kappa_l \delta \left(\frac{1}{2\delta} - \kappa_l \cot(2\kappa_l \delta) \right) + \frac{2\delta}{\pi} \int_{-\infty}^{\infty} d\zeta_+ \, \zeta_+ \ln|a(k)|^2. \tag{6.14b}$$

7. NOTES ON THE BENJAMIN–ONO EQUATION

In Secs. 4–6, we developed a method associated with the IST problem of (1.1) in the case where the Neumann series corresponding to the integral equation (3.4) converges. Sufficient conditions for this to hold are to have δ *finite* and $\max|u|$ chosen small enough (see Appendix B). We now briefly consider the scattering problem in the case $\delta = \infty$, and we find several results associated with the BO equation by solving the scattering problem. Our basic philosophy regarding this case is to obtain information by taking the limit process $\delta \to \infty$.

From (3.2) and (3.3) with $\delta \to \infty$, the IST scheme of the BO equation is given by

$$iw_x^+ + 2k(w^+ - w^-) = -uw^+, \tag{7.1}$$

$$iw_t^\pm - 4ikw_x^\pm + w_{xx}^\pm + [\mp 2iP^\pm(u_x) + \rho]w^\pm = 0, \tag{7.2}$$

where $P^\pm(\cdot)$ are the usual projection operators given by $P^\pm(\cdot) = \frac{1}{2}[1 \mp iH](\cdot)$, and $w^\pm(x)$ are the boundary values of the functions analytic in the upper and lower half z plane, respectively. Here we require that the *derivatives* of $w^\pm(x;k)$ satisfy

$$Hw_x^\pm = \pm iw_x^\pm \tag{7.3}$$

With (3.11) and (3.12), we define the Jost functions of (7.1) as follows. For real $k > 0$,

$$m^\pm(x;k) = \lim_{\delta \to \infty} M^\pm(x;k), \tag{7.4a}$$

$$\bar{m}^\pm(x;k) = \lim_{\delta \to \infty} \bar{M}^\pm(x;k) \exp(-2k\delta), \tag{7.4b}$$

$$n^\pm(x;k) = \lim_{\delta \to T} N^\pm(x;k) \exp(-2k\delta), \tag{7.5a}$$

$$\bar{n}^\pm(x;k) = \lim_{\delta \to \infty} \bar{N}^\pm(x;k). \tag{7.5b}$$

As mentioned in Appendix A, these Jost functions are the solutions of the split equations

$$iw_x^+ + 2k(w^+ - w_0) = -P^+(uw^+), \tag{7.6a}$$

$$2k(w^- - w_0) = P^-(uw^+), \tag{7.6b}$$

where w_0 is a constant determined by the boundary condition. The Green's functions associated with (7.4) and (7.5), defined by $g^\pm_{1,2}(x,y;k) = \lim_{\delta \to \infty} G^\pm_{1,2}(x,y;k)$, are given in the explicit form, for real $k > 0$,

$$g_1^+(x,y;k) = ie^{2ik(x-y)} \left\{ \theta(x-y) - \frac{i}{2\pi} E_i[2ik(x-y)] \right\}, \tag{7.7a}$$

$$g_2^+(x,y;k) = ie^{2ik(x-y)} + g_1^+(x,y;k), \tag{7.7b}$$

$$g_1^-(x,y;k) = \frac{1}{4\pi ik(x-y-i0)}, \tag{7.8a}$$

$$g_2^-(x,y;k) = g_1^-(x,y;k), \tag{7.8b}$$

where $\theta(\cdot)$ is the usual Heaviside step function, and $E_i(z)$ is the exponential integral,

$$E_i(z) = \int_z^\infty \frac{e^{-t}}{t}\, dt, \quad \text{for } |\arg z| < \pi, \tag{7.9}$$

and asymptotically $E_i(z) \to 0(e^{-z}/z)$ as $|z| \to \infty$. The integral equations for m^+ and n^+ are found in the same way as in Sec. 3; hence, from (7.7), we have, for real $k > 0$,

$$m^+(x;k) = 1 + \beta(k)e^{2ikx} + \int_{-\infty}^{\infty} g_2^+(x,y;k)u(y)m^+(y;k)\, dy, \tag{7.10}$$

$$n^+(x;k) = \bar{\alpha}(k)e^{2ikx} + \int_{-\infty}^{\infty} g_1^+(x,y;k)u(y)n^+(y;k)\, dy, \tag{7.11}$$

which leads to

$$m^+(x;k) = \bar{n}^+(x;k) + \beta(k)n^+(x;k), \tag{7.12}$$

$$\bar{n}(x;k) = \bar{\alpha}(k)\bar{m}^+(x;k), \tag{7.13}$$

whenever the solutions of (7.10) *and* (7.11) *are unique.* Here $\beta(k)$ and $\bar{\alpha}(k)$ are given by

$$\beta(k) = \lim_{\delta\to\infty} b(k)\exp(2k\delta) = i\int_{-\infty}^{\infty} u(y)m^+(y;k)e^{-2iky}\,dy, \tag{7.14}$$

$$\bar{\alpha}(k) = \lim_{\delta\to\infty} \bar{a}(k) = 1 - i\int_{-\infty}^{\infty} u(y)n^+(y;k)e^{-2iky}\,dy \tag{7.15}$$

[note that, for real $k>0$, $a(k)\to 1$, $\bar{b}(k)\to 0$ as $\delta\to\infty$]. So far we have discussed the Jost functions for real $k>0$. A remarkable feature of the scattering problem (7.1) may arise for real $k<0$. In this case, the Green functions become

$$g_1^+(x,y;k) = g_2^+(x,y;k) = (1/2\pi)E_i[2ik(x-y)]e^{2ik(x-y)}, \tag{7.16}$$

and $g_{1,2}^-(x,y;k)$ are the same as (7.8). Then, the Jost functions are given by

$$m^+(x;k) = 1 + \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{2ik(x-y)} E_i[2ik(x-y)]u(y)m^+(y;k)\,dy, \tag{7.17}$$

$$n^+(x;k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{2ik(x-y)}E_i[2ik(x-y)]u(y)n^+(y;k)\,dy, \tag{7.18}$$

where we have omitted the term $\exp(2ikx)$ in (3.12a), since this function is not analytic on the upper half z plane ($\mathrm{Re}\, z = x$) for $k<0$ in the sense of (7.3). We note that if there is a nontrivial solution of (7.18), then, by the asymptotics of $E_i(x)$, $n^+(x;k)\to O(1/x)$ as $|x|\to\infty$ [i.e., this solution may be considered to be a bound state for (7.1)]. By the method of successive approximations,[10] one can find that if the kernel $K(x,y;k)\equiv(2\pi)^{-1}E_i[2ik(x-y)]u(y)\exp[2ik(x-y)]$ satisfies the following square integral conditions,

$$S_1(x)\equiv\int_{-\infty}^{\infty} |K(x,y;k)|^2\,dy < \infty,$$
$$S_2(y)\equiv\int_{-\infty}^{\infty} |K(x,y;k)|^2\,dx < \infty, \tag{7.19}$$
$$S_0\equiv\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |K(x,y;k)|^2\,dx\,dy < \infty,$$

and if $S_0<1$, then there is only the trivial solution to (7.18), i.e., $n^+(x;k)=0$. For real k, the condition $S_0<1$ gives

$$\int_{-\infty}^{\infty} [u(x)]^2\,dx < 4\pi|k|. \tag{7.20}$$

This implies that, for given $u(x)$, one may expect to have a nontrivial solution for those k satisfying $|k| < (4\pi)^{-1}\int_{-\infty}^{\infty}[u(x)]^2\,dx$. In order to illustrate some of those features [e.g., the existence of nontrivial solutions of (7.18)] of the scattering problem (7.1), we discuss a simple example. Namely consider the following initial condition,

$$u(x) = \frac{2\nu\epsilon}{x^2+\epsilon^2}, \tag{7.21}$$

where ν and ϵ are constants, and without loss of generality ϵ can be taken 1 by virtue of the scaling asymmetry, $x\to\epsilon x$, $t\to\epsilon^2 t$, $u\to u/\epsilon$ (the BO equation with this initial condition has been discussed numerically in Ref. 11). The method discused below can be applied to the case in which $u(x)$ takes more general form of a rotational function. For a bound state (i.e., real $k<0$), by virtue of Cauchy's theorem, we immediately obtain $n^-(x;k)$, from (7.6b),

$$\begin{aligned} n^-(x;k) &= \frac{1}{2k}P^-(un^+)(x;k) \\ &= \frac{1}{4\pi ik}\int_{-\infty}^{\infty}\frac{1}{x-y-i0}\left(\frac{2\nu}{y^2+1}\right)n^+(y;k)\,dy \\ &= \frac{1}{2k}\mathrm{Res}\left[\frac{1}{x-y-i0}\left(\frac{2\nu}{y^2+l}\right)n^+(y;k)\right] \\ &= -\frac{i\nu n^+(i;k)}{2k(x-i)}, \end{aligned} \tag{7.22}$$

where we have used the requirement that $n^+(y;k)$ is analytic on the upper half plane. It should be noted that $n^-(x;k)$ can be calculated explicitly and the degree of singularity in the upper half plane is the same as the one of $u(x)$ when $u(x)$ is the rational function. Then the solution $n^+(x;k)$ can be found directly from (7.1) in the form

$$\frac{n^+(x;k)}{n^+(i;k)} = -\nu\left(\frac{x-i}{x+i}\right)^{\nu}\int_{-\infty}^{x}\left(\frac{y+i}{y-i}\right)^{\nu} \times\frac{\exp[2ik(x-y)]}{y-i}\,dy, \tag{7.23}$$

with the boundary condition ($n^+(x;k)\to 0$ as $|x|\to\infty$)

$$D_\nu(k)\equiv\int_{-\infty}^{\infty}\left(\frac{y+i}{y-i}\right)^{\nu}\frac{\exp(-2iky)}{y-i}\,dy = 0, \tag{7.24}$$

which determines the discrete eigenvalues (see below). For $\nu<0$, integrating (7.23) by parts, one may see that $n^+(z;k)$ has a singular point at $z=i$, and there is no bound state. As a special case of $\nu>0$, we first consider the case $\nu=n=$ integer. By a residue calculation, one can see that (7.24) is the Laguerre polynomial of degree n, i.e., $D_n(k) = (2\pi i)^{-1}L_n(-4k)\exp(4k) = 0$ for $k<0$. Hence there are n real distinct eigenvalues, e.g., for $n=1$, $k_1 = -\frac{1}{4}$, *for* $n=2$, $k_{1,2} = -(2\pm\sqrt{2})/4$, and so on. On the other hand, (7.23) can be written in the form,

$$\frac{n^+(x;k)}{n^+(i;k)} = -\nu\left(\frac{x-i}{x+i}\right)^{n}e^{2ikx}\left[\sum_{l=0}^{n}\binom{n}{l}(2i)^{n-l}I_l^{(n)}(x;k)\right], \tag{7.25}$$

TABLE I. The eigenvalues of the Fredholm integral equation (7.18).

ν	0.8	1.0	1.5	2.0	2.5	3.0
$-4k$	0.48	1.0	0.12	0.59	0.085	0.42
			1.97	3.41	1.28	2.29
					4.69	6.29

where $I_l^{(n)}(x;k)$ is given by

$$I_l^{(n)}(x;k) = \int_{-\infty}^{x} \frac{\exp(-2iky)}{(y-i)^{n-l+1}}\,dy$$
$$= -\frac{1}{n-l}\left[\frac{\exp(-2ikx)}{(x-i)^{n-l}} - 2ikI_{l+1}^{(n)}(x;k)\right]$$
$$= \cdots\cdots$$
$$= \sum_{m=1}^{n-l} \frac{\gamma_m e^{-2ikx}}{(x-i)^m} + \frac{(-2ik)^{n-l}}{(n-l)!} I_n^{(n)}(x;k). \tag{7.26}$$

Here γ_m is the constant to be calculated recursively, and $I_n^{(n)}(x;k)$ is the exponential integral $E_i[2ik(x-i)]$ which has a logarithmic singularity at $x = i$. However, the coefficient of $I_n^{(n)}$ in $n^+(x;k)$ is just the Laguerre polynomial, i.e.,

$$L_n(-4k) = \sum_{l=0}^{n} \binom{n}{l} \frac{(4k)^{n-l}}{(n-l)!}, \tag{7.27}$$

which is required to be zero by the condition (7.24). Namely, the condition (7.24) corresponds to the requirement that $n^+(x;k)$ is, in fact, analytic in the upper half plane. Thus we expect to find an n-soliton solution when $\nu = n$ (in agreement with Ref. 11). By direct calculations, one can show that the solution (7.25) with (7.27) = 0 satisfies (7.18) [i.e., this shows the existence of the nontrivial solution to the homogeneous integral equation (7.18)]. For the situation with $\nu \neq$ integer, we note that (7.24) can be expressed by

$$(1 - e^{2\pi i\nu}) \int_0^{\infty} \frac{(y+l)^{\nu} e^{4ky} - \sum_{l=0}^{[\nu]} \alpha_l y^l}{y^{l+\nu}}\,dy = 0, \tag{7.28}$$

where $[\nu]$ denotes the Gauss's symbol (i.e., maximum integer less than ν), and the series $\Sigma_{l=0}^{[\nu]} \alpha_l y^l$ is the first $[\nu] + 1$ terms of the Taylor expansion of $(y+1)^{\nu} \exp(4ky)$ around $y = 0$. From (7.28), we find that there are n roots of (7.28) when ν is in the range $n - 1 < \nu \leqslant n$. We have listed the values of k versus ν in Table I.

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APPENDIX A: GREEN'S FUNCTIONS

We give here the form of the Green's function $G^{\pm}(x,y;k)$ in the limits of $\delta \to 0$ and $\delta \to \infty$ for real k.

For $\delta \to 0$, taking $\zeta_+ \to k$ into account, the Green's function (3.6) with (3.7) becomes

$$G(x,y;k) \to \frac{1}{2\pi\delta} \int_C \frac{e^{ip(x-y)}}{p(p-2k)}\,dp, \tag{A1}$$

which is the Green's function of the Schrödinger equation of $V(x;k) = \lim_{\delta \to 0} W(x;k)$, i.e.,

$$\delta(V_{xx} + 2ikV_x) + uV = 0 \tag{A2}$$

[note $V = \phi \exp(-ikx)$ where ϕ is in (2.7)]. On the other hand, for $\delta \to \infty$, we have

$$\hat{G}(p;k) \to \frac{1}{p-2k}\,\theta(p), \tag{A3a}$$

$$\hat{G}^{-}(p;k) \to \frac{1}{2k}\,\theta(p), \tag{A3b}$$

where $\theta(\cdot)$ is the usual Heaviside step function. It should be noted that $\zeta_+(k) \to 2k\theta(k)$ for real k, and the negative eigenvalue in (7.1) corresponds to what happens to $\zeta_+ < -1/(2\delta)$ (i.e., k is on the edge of the PB) for finite δ. From (A3), we have

$$G^{+}(x,y;k) \to \frac{1}{2\pi} \int_{C^+} \frac{e^{ip(x-y+i0)}}{p-2k}\,dp, \tag{A4a}$$

$$G^{-}(x,y;k) \to \frac{1}{4\pi k} \int_{-\infty}^{0} e^{-ip(x-y-i0)}\,dp, \tag{A4b}$$

where the contour C^+ is taken to be a positive half p line avoiding the singularity $p = 2k$ (see Sec. 7). It is remarkable that (A4b) is just the usual projection operator $P^{-}(\cdot) = \frac{1}{2}(1 + iH)(\cdot)$, i.e.,

$$G^{-}(x,y;k) \to \frac{1}{4\pi ik(x-y-i0)}$$
$$= \frac{1}{4k}\left[\delta(x-y) - \frac{i}{\pi} P \frac{1}{x-y}\right]$$
$$= \frac{1}{2k}\hat{P}^{-}(x-y) \tag{A5}$$

[note that $P^{-}(\cdot) = \int_{-\infty}^{\infty} dy\, \hat{P}^{-}(x-y)(\cdot)$]. Indeed, the Green's functions $G^{\pm}(x,y;k)$ decompose the scattering problem into two equations:

$$iG_x^{+}(x,y;k) + (\zeta_+ + 1/2\delta)G^{+}(x,y;k) = -\Delta^{+}(x-y), \tag{A6a}$$

$$(\zeta_+ + 1/2\delta)G^{-}(x,y;k) = \Delta^{-}(x-y), \tag{A6b}$$

where the functions $\Delta^{\pm}(x-y)$ satisfying $\Delta^{+}(x-y) + \Delta^{-}(x-y) = \delta(x-y)$ (i.e., $\Delta^{\pm}$ is a decomposition of δ-function) are given by

$$\Delta^{+}(x-y) = \frac{1}{2\pi} \int_C dp\, \frac{p - (\zeta_+ + 1/2\delta)}{p - (\zeta_+ + 1/2\delta)(1 - e^{-2\delta p})}\, e^{ip(x-y+i0)}, \tag{A7a}$$

$$\Delta^{-}(x-y) = \frac{1}{2\pi} \int_C dp\, \frac{(\zeta_+ + 1/2\delta)e^{-2\delta p}}{p - (\zeta_+ + 1/2\delta)(1 - e^{-2\delta p})}\, e^{ip(x-y-i0)}. \tag{A7b}$$

Here we note that for $\delta \to \infty$, (A7) tend to the usual projection operators,

$$\Delta^{\pm}(xy) \to \hat{P}^{\pm}(x-y) = \frac{\pm i}{2\pi(x-y \pm i0)}. \tag{A8}$$

APPENDIX B: ANALYTICITY OF THE JOST FUNCTIONS

Here we discuss the analytical property of $M^{+}(x;k)$ in the fundamental sheet (FS). [The analyticity of $\bar{N}^{+}(x;k)$ can be discussed in a similar fashion to that considered here.] In order to do this, it is convenient to write $G_1^{+}(x,y;k)$ in the explicit form calculated by the residue theorem, i.e.,

$$G_1^+(x,y;k) = \frac{i}{2\delta}\sum_{n=-1}^{\infty}\frac{1}{p_n-\zeta_+}\exp[ip_n(x-y)]\theta(x-y) - \frac{i}{2\delta}\sum_{n=1}^{\infty}\frac{1}{\bar{p}_n-\zeta_+}\exp[i\bar{p}_n(x-y)]\theta(y-x). \tag{B1}$$

Here p_n $(n\geqslant -1)$, $\bar{p}_n$ $(n\geqslant 1)$ are given below (3.7).

Firstly, we show that in the upper half plane of the FS, $G_1^+(x,y;k)$ [and therefore $M^+(x;k)$] is holomorphic at the points on the branch cut corresponding to the edge of the principal branch (PB) in $\mathrm{Im}\, k>0$.

Let ζ_{+o} be the point on the branch cut in the upper half plane of the FS. Then there are two points k_1, k_2 (say, $\mathrm{Re}\, k_1 < \mathrm{Re}\, k_2$) on the edge of the PB, such that $\zeta_{+o}(k_1) = \zeta_{+o}(k_2)$. Calculating the two limits of $G_1^+(x,y;k)$ in the FS (or PB),

$$\lim_{\substack{\mathrm{Im}\,\zeta_+\downarrow \mathrm{Im}\,\zeta_{+o}\\ \zeta_+\to\zeta_{+o}}} G_1^+(x,y;k) = \lim_{k\to k_1} G_1^+(x,y;k) \tag{B2a}$$

and

$$\lim_{\substack{\mathrm{Im}\,\zeta_+\uparrow \mathrm{Im}\,\zeta_{+o}\\ \zeta_+\to\zeta_{+o}}} G_1^+(x,y;k) = \lim_{k\to k_2} G_1^+(x,y;k), \tag{B2b}$$

we obtain (B2a) = (B2b), since at k_1, $p_0=2k_1$, $p_1=2k_2$, at k_2, $p_0=2k_2$, $p_1=2k_1$, and the other poles p_n, $\bar{p}_n$ $(n\geqslant 2)$ remain the same. Hence, $G_1^+(x,y;k)$ does not have the branch cut in the upper half plane of the FS. It should be noted that for $\mathrm{Im}\,\zeta_+<0$, $G_1^+(x,y;k)$ has a branch cut corresponding to the lower edge of the PB. For $G_2^+(x,y;k)$ [associated with $\bar{N}(x;k)$], similar reasoning suggests that $G_2^+(x,y;k)$ does not have the branch cut in the lower half plane of the FS.

Now let us discuss the analyticity of $M^+(x;k)$ for $\mathrm{Im}\,\zeta_+\geqslant 0$. In the case $\zeta_+\neq p_n$ $(n\geqslant 0)$ (i.e., there is no double zero), one can estimate, from (B1),

$$\int_{-\infty}^{\infty}|G_1^+(x,y;k)u(y)|\,dy \leqslant \frac{1}{2\delta}\left(\frac{1}{|\zeta_+|}+\frac{1}{|\zeta_-|}\right)\int_{-\infty}^{\infty}|u(y)|\,dy + \frac{2\max|u|}{\pi}\sum_{n=1}^{\infty}\frac{1}{(2n-1)|p_n-\zeta_+|} \equiv \alpha_1<\infty. \tag{B3}$$

(i.e., the kernel can be estimated by a constant which depends on δ, $\max|u|$ and $\int_{-\infty}^{\infty}|u|\,dx$). Then, by the method of successive approximation, we have the Neumann series for $|M^+(x;k)|$ in the form

$$|M^+(x;k)|\leqslant 1+\int_{-\infty}^{\infty}|G_1(x,y;k)u(y)|\,dy + \int_{-\infty}^{\infty}dy_1\int_{-\infty}^{\infty}dy_2|G_1(x,y_1;k)u(y_1)G_1(y_1,y_2;k)u(y_2)| + \cdots \leqslant 1+\alpha_1+\alpha_1^2+\cdots. \tag{B4}$$

If $\alpha_1(k,\delta)$ is less than 1, then (B4) converges and $|M^+(x;k)|$ is uniformly bounded. For the case, $p_{n_0}=p_{n_0+1}=\zeta_+$ $(n\geqslant 0)$ for a certain n_0 (i.e., there is a double zero in the upper half plane of the FS), we have

$$\int_{-\infty}^{\infty}|G_1^+(x,y;k)u(y)|\,dy \leqslant \frac{1}{|2n_0-1|\pi}\int_{-\infty}^{\infty}|u(y)|\,dy + \frac{2\delta\max|u|}{\pi}\left[\frac{1}{\delta}\sum_{n=0}^{\infty}{}'\frac{1}{|2n-1||p_n-p_{n_0}|} + \frac{4}{3|2n_0-1|}+\frac{6}{(2n_0-1)^2\pi}\right]\equiv\alpha_2<\infty, \tag{B5}$$

where $\Sigma'^{\infty}_{n=0}$ expresses the sum over $n\geqslant 0$ except $n=n_0$ and n_0+1. Thus, the convergence of the Neumann series is given by $\alpha_2<1$, and $|M^+(x;k)|$ is also uniformly bounded. In the case $\zeta_+=0$ $(k=0)$, we need a different way to estimate $|M^+(x;k)|$. Here the estimation of the kernel $G_1^+(x,y;k)u(y)$ depends on x. We write the integral equation for $M^+(x;k)$ in the form

$$M^+(x;k) = 1+\int_{-\infty}^{x}V(x,y;k)u(y)M^+(y;k)\,dy + \int_{-\infty}^{\infty}F(x,y;k)u(y)M^+(y;k)\,dy. \tag{B6}$$

where

$$V(x,y;k) = \frac{1}{2i\delta\zeta_+} - \frac{1}{2i\delta\zeta_-}e^{2ik(x-y)}, \tag{B7a}$$

$$F(x,y;k) = G_1^+(x,y;k) - V(x,y;k). \tag{B7b}$$

Define $\Phi(x;k)$ to be

$$\Phi(x;k) = 1+\int_{-\infty}^{\infty}F(x,y;k)u(y)M^+(y;k)\,dy, \tag{B8}$$

from which we have

$$M^+(x;k) = \Phi(x;k)+\int_{-\infty}^{x}V(x,y;k)u(y)M^+(y;k)\,dy. \tag{B9}$$

Noting that (B9) is a Volterra integral equation, we have a resolvent kernel $\Gamma(x,y;k)$ given by

$$\Gamma(x,y;k) = \sum_{n=1}^{\infty}K^{(n)}(x,y;k), \tag{B10}$$

with

$$K^{(n)}(x,y;k) = \int_y^x ds\, V(x,s;k)K^{(n-1)}(s,y;k),$$

$$K^{(1)}(x,y;k) = V(x,y;k)u(y), \tag{B11}$$

and $M^+(x;k)$ is given by

$$M^+(x;k) = \Phi(x;k)+\int_{-\infty}^{x}\Gamma(x,y;k)\Phi(y;k)\,dy. \tag{B12}$$

From (B12), (B8) can be written as a Fredholm integral equation in the form

$$\Phi(x;k) = 1+\int_{-\infty}^{\infty}K(x,y;k)\Phi(y;k)\,dy, \tag{B13}$$

whose kernel

$$K(x, y;k) = F(x, y;k)u(y) + \int_y^\infty F(x,s;k)u(s)\Gamma(s, y;k)\, ds \tag{B14}$$

[note that $F(x, y;k)$ (and therefore $K(x, y;k)$] has a logarithmic singularity at $x = y$. By the method of successive approximations for (B13), if $K(x, y;k)$ satisfies the following conditions,[10]

$$\int_{-\infty}^{\infty} |K[x, y;k)|^2\, dy = \beta_1(x) < \infty, \quad \text{for all } x, \tag{B15a}$$

$$\int_{-\infty}^{\infty} |K(x, y;k)|^2\, dx \equiv \beta_2(y) < \infty, \quad \text{for all } y, \tag{B15b}$$

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |K(x, y;k)|^2\, dx\, dy < 1, \tag{B15c}$$

then the Neumann series of (B13) converges. In the case $k = 0$, we have the estimation $|K(x, y;0)|$, for $x \neq y$,

$$|K(x, y;0)| \leqslant |F(x, y;0)u(y)| + \frac{1}{2\pi}|u(y)|\int_{-\infty}^{\infty} ds |F(x,s;0)u(s)\Gamma(s, y;0)|\, ds \tag{B16}$$

with

$$|\Gamma(x, y;0)| \leqslant \frac{2}{3}\left[1 + \frac{3}{2\delta}(|y| + |x|)\right] \times \exp\left[\beta + \frac{1}{\delta}x\theta(x)\int_{-\infty}^{\infty}|u(s)|ds\right], \tag{B17}$$

$$|F(x, y;0)| \leqslant \frac{1}{2\delta}\sum_{n=1}^{\infty}\frac{1}{|p_n|}\exp\left[-\frac{(2n-1)\pi}{2\delta}|x - y|\right] \leqslant \frac{1}{2\pi}\ln\frac{1 + \exp[-(\pi/2\delta)|x - y|]}{1 - \exp[-(\pi/2\delta)|x - y|]}, \tag{B18}$$

$$\beta = \frac{2}{3}\int_{-\infty}^{\infty}\left(1 + \frac{34}{2\delta}|x|\right)|u(x)|\, dx. \tag{B19}$$

From (B16), one can see that, for finite δ, if $u(x)$ decays sufficiently rapidly as $|x| \to \infty$, then $|K(x, y;0)|$ is square integrable. Moreover the Neumann series converges for given δ and $\max|u|$ chosen small enough. Namely, the solution of (B13) exists for all x, and therefore $M^+(x,0)$ exists. It is interesting to note that, for the limit $\delta \to 0$ with $u(x)/\delta$ remaining finite, $F(x, y;k)$ tends to zero and (B6) becomes the Volterra equation of the Schrödinger equation (see Appendix A). Consequently, these results imply that $M^+(x;k)$ is analytic in the upper half plane of the FS whenever the Neumann series converges in this region.

APPENDIX C: RELATIONS BETWEEN $\{a(k),b(k)\}$ and $\{\bar{a}(k),\bar{b}(k)\}$

For real k, we derive the relations (3.22) and (3.23). In order to do this, it is convenient to consider the following form of the scattering problem,

$$i\phi_x^+ + \left(u + \frac{1}{2\delta}\right)\phi^+ = \Gamma(k)\phi^-, \tag{C1}$$

where

$$\phi(x;k) \equiv W(x;k)\exp(-i\zeta_+ x),$$

and $\Gamma(k) \equiv (\zeta_+ + 1/2\delta)\exp(-2\delta\zeta_+) = (-\zeta_- + 1/2\delta)\exp(2\delta\zeta_-) = \Gamma(-k)$. Then, for real k, the Jost functions are defined by

$$f(x,k) \to e^{-i\zeta_+ x}, \quad \text{as } x \to -\infty, \tag{C2a}$$

$$g(x;k) \to e^{i\zeta_- x}, \quad \text{as } x \to +\infty, \tag{C2b}$$

[note that from $\Gamma(k) = \Gamma(-k)$, if $\phi(x;k)$ is a solution, then $\phi(x;-k)$ is also a solution]. Then the relations (3.20) and (3.21) become

$$f(x;k) = a(k)g(x;-k) + b(k)g(x;k), \tag{C3}$$

$$g(x;k) = \bar{a}(k)f(x;-k) + \bar{b}(k)f(x;k), \tag{C4}$$

from which we have

$$a(k)\bar{a}(-k) + b(k)\bar{b}(k) = 1, \tag{C5a}$$

$$\bar{a}(k)a(-k) + b(k)\bar{b}(k) = 1, \tag{C5b}$$

and

$$a(k)\bar{b}(-k) + b(k)\bar{a}(k) = 0, \tag{C6a}$$

$$\bar{a}(k)b(-k) + \bar{b}(k)a(k) = 0. \tag{C6b}$$

On the other hand, from (C1) and its complex conjugate equation, we have

$$i\frac{\partial}{\partial x}[\phi^+\{\phi^+\}^*] = \Gamma[\phi^-\{\phi^+\}^* - \{\phi^-\}^*\phi^+]. \tag{C7}$$

By virtue of the relation $[\phi^{\pm}]^* = [\phi^*]^{\mp}$, we obtain

$$0 = i[\phi^+\{\phi^*\}^-]\Big|_{x=-\infty}^{x=\infty} + \Gamma(k)\lim_{l\to\infty}\left(\int_{-l-i\delta}^{-l+i\delta}dx + \int_{l-i\delta}^{l+i\delta}dx\right)|\phi|^2. \tag{C8}$$

Using $f(x;k)$ as $\phi(x;k)$ in (C8), and taking the boundary condition of $f(x;k)$ into account, we obtain (3.23). Also comparing (3.23) with (C5) and (C6), we have (3.22).

APPENDIX D: BOUND STATES

Here we show that the zeroes of $a(k)$ are pure imaginary and simple.

From (2.1), we have

$$i\frac{\partial}{\partial x}[\psi_1^+\{\psi_1^+\}^*] - (\lambda_1 - \lambda_1^*)[\psi_1^+\{\psi_1^+\}^*] = \mu_1\psi_1^-\{\psi_1^+\}^* - \mu_1^*\psi_1^+\{\psi_1^-\}^*, \tag{D1}$$

where $\psi_1 \equiv (x;k_1)$, $\lambda_1 = \lambda(k_1)$, $\mu_1 = \mu(k_1)$ and $\mathrm{Im}\, k_1 > 0$. By virtue of that $[\psi^{\pm}]^* = [\psi^*]^{\mp}$, we have

$$(\lambda_1 - \lambda_1^*)\int_{-\infty}^{\infty}|\psi_1^+|^2\, dx + (\mu_1 - \mu_1^*)\int_{-\infty}^{\infty}|\psi_1|^2\, dx = 0. \tag{D2}$$

From (D2), using the formula of λ and μ in terms of the k [see below (2.2)], we obtain $k_1 = i\kappa_1$.

In order to prove $a(k_1) \neq 0$ (i.e., k_1 is a simple), we show the following relation, for the bound state $k = i\kappa$,

$$C^{-1} \equiv i\dot{a}/b = \int_{-\infty}^{\infty}|g(x;i\kappa)|^2\, dx, \tag{D3}$$

where $g(x;i\kappa)$ is given by (C2b), and C is defined in (4.8). From

(C1) and its derivative with respect to ζ_+, i.e.,

$$i\dot{\phi}_x^+ + (u + 1/2\delta)\dot{\phi}^+ = \Gamma\dot{\phi}^- + \dot{\Gamma}\phi^- \qquad \text{(D4)}$$

[here the dot denotes the derivative with respect to ζ_+, e.g., $\dot{\Gamma} = -2\delta\zeta_+ \exp(-2\delta\zeta_+)$], we have, for $k = i\kappa$,

$$i\frac{\partial}{\partial x}[\dot{\phi}^+\{\phi^+\}^*] = \Gamma[\dot{\phi}^-\{\phi^+\}^* - \dot{\phi}^+\{\phi^-\}^*] - 2\delta\zeta_+ e^{-2\delta\zeta_+}\phi^-\{\phi^+\}^*, \qquad \text{(D5)}$$

where $\dot{\phi} = \partial\phi/\partial\zeta_+|_{k=i\kappa}$, and we have used $\Gamma^*(i\kappa) = \Gamma(i\kappa)$. Integrating (D5) over $-\infty$ to ∞, we have

$$i\dot{\phi}^+\{\phi^+\}^*|_{x=-\infty}^{x=\infty} = \Gamma\lim_{l\to\infty}\left(\int_{-l+i\delta}^{-l-i\delta}dx + \int_{l-i\delta}^{l+i\delta}dx\right)\dot{\phi}\phi^*$$
$$-2\delta_+e^{-2\delta\zeta_+}\lim_{l\to\infty}\left(\int_{-l+i\delta}^{-l}dx + \int_{-l}^{l}dx + \int_{l}^{l+i\delta}dx\right)|\phi|^2, \qquad \text{(D6)}$$

where we have used $[\phi^{\pm}]^* = [\phi^*]^{\mp}$. From (D6) with $\phi = f$ and the boundary condition of f, we have

$$i\dot{a}b^* = \int_{-\infty}^{\infty}|f(x;i\kappa)|^2\,dx. \qquad \text{(D7)}$$

Consequently, from $f(x;i\kappa) = bg(x;i\kappa)$, we obtain (D3).

APPENDIX E: CLOSURE OF THE JOST FUNCTIONS

Under the condition of the analyticity for the Jost functions considered in Secs. 4–6, we show that the set of the Jost functions defined in (3.11) or (3.12) consists of the closure for the eigenvalue problem (3.2). We use the scattering problem (C1) for convenience.

Let us define the adjoint problem of (C1) in the form

$$-i\{\phi^A\}_x^- + (u + 1/2\delta)\{\phi^A\}^- = \Gamma(k)\{\phi^A\}^+, \qquad \text{(E1)}$$

where $\phi^A = \phi^A(x;k)$ is the adjoint solution of $\phi(x;k)$. For real k, the Jost functions of (E1) are given by

$$f^A(x;k) \to e^{-i\zeta_- x}, \quad \text{as } x\to-\infty, \qquad \text{(E2a)}$$
$$g^A(x;k) \to e^{i\zeta_+ x}, \quad \text{as } x\to+\infty. \qquad \text{(E2b)}$$

From (C2) and (E2), one can see that

$$\phi^A(x;k) = \phi^*(x,-k) \quad \text{for real } k. \qquad \text{(E3)}$$

By virtue of the analytical continuation, we have

$$\phi^A(x;k) = \phi^*(x,-k^*) \quad \text{for complex } k. \qquad \text{(E4)}$$

Let $\langle k|k'\rangle$ be an inner product defined by

$$\langle k|k'\rangle \equiv \int_{-\infty}^{\infty}\phi(x;k)\phi^A(x;k')\,dx \equiv \int_{-\infty}^{\infty}\langle k|x\rangle\langle x|k'\rangle\,dx, \qquad \text{(E5)}$$

where the Dirac symbols are defined by $\langle k|x\rangle \equiv \phi(x;k)$ and $\langle x|k\rangle \equiv [\langle k|x\rangle]^A = \phi^A(x;k)$. Then for real k, from (C1) and (E1), we have

$$[\Gamma(k) - \Gamma(k')]\langle k|k'\rangle = i[\phi^+(k)\{\phi^A(k')\}^-]|_{x=-\infty}^{x=\infty}$$
$$-\Gamma(k)\lim_{l\to\infty}\left(\int_{-l+i\delta}^{-l}dx + \int_{l}^{l+i\delta}dx\right)\phi(k)\phi^A(k')$$
$$+\Gamma(k')\lim_{l\to\infty}\left(\int_{-l-i\delta}^{-l}dx + \int_{l}^{l-i\delta}dx\right)\phi(k)\phi^A(k'). \qquad \text{(E6)}$$

Defining

$$\left.\begin{aligned} f(x,k) &\equiv \langle k,1|x\rangle \quad \text{(E7a)}\\ g(x,k) &\equiv \langle k,2|x\rangle \quad \text{(E7b)}\end{aligned}\right\},$$

and by virtue of the boundary conditions of f and g, we have the following orthogonality relations,

$$\langle k,1|k',2\rangle = 2\pi a(k)\delta(\zeta_+ - \zeta'_+) \quad \text{for real } k,k', \qquad \text{(E8a)}$$
$$\langle k,1|i\kappa_l,2\rangle = \langle i\kappa_l,1|k,2\rangle = 0 \quad \text{for real } k, \qquad \text{(E8b)}$$
$$\langle i\kappa_l,1|i\kappa_m,2\rangle = i\dot{a}_l\delta_{lm}. \qquad \text{(E8c)}$$

If the set of the functions $[\{f(x;k), -\infty<k<\infty\}, \{f(x;i\kappa_l)\}_{l=1}^N]$ is complete in the sense of $L_2(-\infty<x<\infty)$, then an arbitrary function $h(x)$ in L_2 can be expanded in the following form (that is, the expansion theorem),

$$h(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}d\zeta_+\hat{h}(k)f(x;k) + \sum_{l=1}^N h_l f(x;i\kappa_l), \qquad \text{(E9)}$$

where $\hat{h}(k)$ and h_l are determined by using (E8), i.e.,

$$\hat{h}(k) = \frac{1}{a(k)}\int_{-\infty}^{\infty}h(x)g^A(x;k)\,dx, \qquad \text{(E10a)}$$

$$h_l = \frac{1}{i\dot{a}_l}\int_{-\infty}^{\infty}h(x)g^A(x;i\kappa_1)\,dx. \qquad \text{(E10b)}$$

In order to verify the expansion theorem (E9) it is sufficient to show that, for this case, there is an identity operator given in the form[12]

$$I = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\zeta_+}{a(k)}|k,2\rangle\langle k,1| + \sum_{l=1}^N\frac{1}{i\dot{a}_l}|i\kappa_l,2\rangle\langle i\kappa_l,1|, \qquad \text{(E11)}$$

or

$$\begin{aligned}\langle y|I|x\rangle &= \delta(x-y)\\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\zeta_+}{a(k)}g^A(y;k)f(x;k)\\ &\quad + \sum_{l=1}^N\frac{1}{i\dot{a}_l}g^A(y;i\kappa_l)f(x;i\kappa_l)\\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}g^A(y;k)g(x;-k)\,d\zeta_+\\ &\quad + \frac{1}{2\pi}\int_{-1/2\delta}^{\infty}\frac{b(k)}{a(k)}g^A(y;k)g(x;k)\,d\zeta_+\\ &\quad + \sum_{l=1}^N C_l g^A(y;i\kappa_l)g(x;i\kappa_l). \end{aligned} \qquad \text{(E12)}$$

By using the triangular representation of

$$N(x;k) = g(x;k)\exp(i\zeta_+ x),$$

$$g(x;k) = e^{i\zeta_- x} + \int_x^{\infty}K(x,s)e^{i\zeta_- s}\,ds, \qquad \text{(E13)}$$

(E12) becomes

$$\langle y|Ix\rangle = \delta(x-y) + K(x,y) + F(x,y) + \int_x^\infty K(x,s)F(s,y)\,ds + \int_y^\infty K^*(y,s)\Big[K(x,s) + F(x,s) + \int_x^\infty K(x,t)F(t,s)dt\Big]\,ds. \tag{E14}$$

By virtue of the Gel'fand–Levitan equation (4.9), we have

$$\langle y|I|x\rangle = \delta(x-y). \tag{E15}$$

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Parabolic approximations to the time-independent elastic wave equation

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A splitting matrix method is used to derive two parabolic-approximation partial differential equations to the three-dimensional, linear, elastic wave equation in isotropic, inhomogeneous media. The derivation is valid for media whose Lamé parameters vary slowly on the length scale of the wavelength of the elastic waves. Next an integral form of the full wave equation is derived based on the splitting matrix and the parabolic approximation solution. Iteration of this equation gives a three-dimensional vector-valued series which generalizes the one-dimensional Bremmer series (which was used in the study of second-order ordinary differential equations). These results are expected to have applications to geophysical modeling and nondestructive evaluation.

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1. INTRODUCTION

Parabolic or forward-scattering approximations to the reduced scalar wave equation[1–7] have been used extensively in the study of acoustic and electromagnetic wave propagation in inhomogeneous media. The parabolic approximation provides a full wave approximation (including diffraction effects) that is amenable to numerical investigations. It has provided the basis for accurate simulation of wave propagation in media with complicated inhomogeneities, including stochastic media. A recent review of parabolic approximations to the scalar wave equation, including numerous references, can be found in Ref. 6, where important new results on improved parabolic approximations to the reduced scalar wave equation are also presented.

Roughly speaking, the parabolic approximation is used when a particular direction is singled out in a medium by the nature of the excitation of the medium and when it is valid to assume that the dominant behavior of the propagation lies along this distinguished direction. A distinguished direction is defined, for example, by the axis of a pencil of light shining into a piece of glass. The direction is distinguished by the excitation, not by the medium. Thus, it is not necessary to assume that the medium is stratified. The propagation is dominated by behavior along the distinguished direction if the medium is such that the reflections of the incoming wave back along the distinguished direction are negligible. Typically, in the scalar case this situation obtains if the inhomogeneities are small and slowly varying on the length scale of the wavelength of the incoming wave. The parabolic approximation is valid in the vicinity of the axis of the incoming pencil, typically an acute cone with axis coincident with that of the pencil. It is not, however, a uniform approximation along the distinguished direction.

Intuitively there should be, in the appropriate region, a parabolic approximation to the elastic wave equation. Surprisingly in view of the success of such approximations in the scalar case, there have been few attempts to derive such a result. For example, the problem of diffraction in inhomogeneous elastic media was studied both earlier and more thoroughly[8] than parabolic approximations. For the full three-dimensional problem, Ref. 9 provides a parabolic approximation in the case of nearly compressional or nearly shear waves when each component of displacement oscillates at the same spatial frequency. In Ref. 10 an alternate parabolic approximation was derived. In two dimensions, a parabolic approximation in terms of the velocity potentials was derived in Ref. 11.

In this work, parabolic approximations to the three-dimensional elastic wave equation for propagation in inhomogeneous media are derived. The method used is a generalization of the splitting method used for the reduced scalar wave equation in Ref. 5. This method provides a parabolic approximation in both senses of the distinguished direction together with the coupling between waves propagating in either direction. It leads simply to an integral equation equivalent to the full elastic wave equation, including natural boundary conditions. The iterates of the integral equation supply corrections to the parabolic approximation.

The origin of the method developed in Ref. 5 and used here is found in Bremmer's analysis of upward and downward-moving waves modeled by second-order ordinary differential equations.[1] The series that arises from iteration of the above-mentioned integral equation is the generalization of the Bremmer series for the ordinary differential equation (o.d.e.) case. The integral equation itself is a generalization of the Bellman–Kalaba equation,[2] again originally derived for the o.d.e. case and extended to the three-dimensional scalar Helmholtz equation in Ref. 5.

The plan of this paper is the following. Section 2 contains the derivation of parabolic approximations to the elastic wave equation based on splitting methods. In Sec. 3, a heuristic justification of the method, particularly of one of the splittings in Sec. 2, is given. In Sec. 4 an integral equation is derived which yields the generalized Bremmer series. It is fully equivalent to the elastic wave equation together with natural boundary conditions. The iteration of this equation yields corrections to the parabolic approximation. Section 5 compares the results of this paper with those in Ref. 9 and

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gives a brief discussion of the methods and results of this work.

2. DERIVATION OF THE PARABOLIC APPROXIMATIONS

In this section two parabolic approximations for the linear, monochromatic elastodynamic wave equation in an isoptropic, inhomogeneous, elastic medium will be derived. The wave equation in this case is given by

$$(\lambda + 2\mu)\nabla(\nabla\cdot\mathbf{u}) + (\nabla\lambda)(\nabla\cdot\mathbf{u}) - \mu\nabla\times(\nabla\times\mathbf{u}) + (\nabla\mu)\times(\nabla\times\mathbf{u}) + 2[(\nabla\mu)\cdot\nabla]\mathbf{u} + \rho\omega^2\mathbf{u}(\mathbf{r}) = 0, \tag{2.1}$$

where λ and μ are the Lamé parameters, ρ is the mass density, $\mathbf{r}\in R^3$ is a point in the elastic medium, and $\mathbf{u}(\mathbf{r})$ is the elastic wave displacement. The splitting method used in Ref. 5 to derive the Fock (and other) parabolic approximations to the scalar Helmholtz equation will be generalized and applied to Eq. (2.1). Although the logic is straight forward, the tensor structure of elastodynamics leads to a number of complications. For this reason, the derivation will first be outlined.

The first step is to express each component of $\mathbf{u}$ in its approximate "upward" and "downward" projections, denoted as $u_j^{\pm}(\mathbf{r})$ for $j = 1,2,3$. This decomposition, or splitting, is made for physical reasons. The reader is referred to Refs. 4 and 5 for a discussion of these arguments. Additional heuristic arguments for the decomposition used here will appear in Sec. 3. Suppose that the coordinate axes are chosen such that the distinguished direction in R^3 is x_1 with x_2 and x_3 as the other two orthogonal coordinate axes. In the notation where partial differentiation of u_j with respect to x_1 is written as

$$(u_{j,x_1})(\mathbf{r}) \equiv \left(\frac{\partial u_j}{\partial x_1}\right)(\mathbf{r}),$$

the quantities $u_j^{\pm}$ will always be linear combinations of u_j and u_{j,x_1}. The second step is to rewrite the original wave equation as a system of first order in x_1 for the variables $u_j^{\pm}$. It is emphasized that this system is *equivalent* to the original second-order wave equation. It re-expresses the physical content of the wave equation, Eq. (2.1), in variables which are interpreted as upward and downward moving waves in the x_1 direction. Each approximate upward and downward wave component is then written as an amplitude function $v_j^{\pm}$ times the exponential of a fast phase. In general the fast phases are different in different components. Next, the equations for the $v_j^{\pm}$'s are derived. Then it is assumed that the coupling between up- and down-moving waves can be neglected to first order in the approximation. The interpretation of the neglected terms as reflections is consistent with the interpretation of the $u_j^{\pm}$'s. The resulting equations are the parabolic approximation to the elastic wave equation.

To implement this procedure it is useful to rewrite Eq. (2.1) in the equivalent component form as

$$\frac{\partial}{\partial x_1}\left[(\lambda + 2\mu)\frac{\partial u_1}{\partial x_1} + \lambda\left(\frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\right)\right] + \frac{\partial}{\partial x_2}\left[\mu\left(\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}\right)\right] + \frac{\partial}{\partial x_3}\left[\mu\left(\frac{\partial u_1}{\partial x_3} + \frac{\partial u_3}{\partial x_1}\right)\right] + \rho\omega^2 u_1(\mathbf{r}) = 0, \tag{2.2}$$

plus two other equations obtained from cyclic permutations of 123 in Eq. (2.2).

These equations can be rewritten as

$$\frac{\partial}{\partial x_1}[\mathbf{u},_{x_1}] = K\cdot u\mathbf{u} + L\cdot\mathbf{u},_{x_1}, \tag{2.3}$$

where the matrix operators K and L,

$$K = (k_{ij}), \tag{2.4}$$

$$L = (l_{ij}), \tag{2.5}$$

are given by

$$k_{11} = -(\lambda + 2\mu)^{-1}\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right) + \frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right) + \rho\omega^2\right], \tag{2.6a}$$

$$k_{12} = -(\lambda + 2\mu)^{-1}\left[\left(\frac{\partial\lambda}{\partial x_1}\right)\left(\frac{\partial}{\partial x_2}\cdot\right)\right], \tag{2.6b}$$

$$k_{13} = -(\lambda + 2\mu)^{-1}\left[\left(\frac{\partial\lambda}{\partial x_1}\right)\left(\frac{\partial}{\partial x_3}\cdot\right)\right], \tag{2.6c}$$

$$k_{21} = -\mu^{-1}\left[\left(\frac{\partial\mu}{\partial x_1}\right)\left(\frac{\partial}{\partial x_2}\cdot\right)\right], \tag{2.6d}$$

$$k_{22} = -\mu^{-1}\left[\frac{\partial}{\partial x_2}\left((\lambda + 2\mu)\frac{\partial}{\partial x_2}\cdot\right) + \frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right) + \rho\omega^2\right], \tag{2.6e}$$

$$k_{23} = -\mu^{-1}\left[\frac{\partial}{\partial x_2}\left(\lambda\frac{\partial}{\partial x_3}\cdot\right) + \frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)\right], \tag{2.6f}$$

$$k_{31} = -\mu^{-1}\left[\left(\frac{\partial\mu}{\partial x_1}\right)\left(\frac{\partial}{\partial x_3}\cdot\right)\right], \tag{2.6g}$$

$$k_{32} = -\mu^{-1}\left[\frac{\partial}{\partial x_3}\left(\lambda\frac{\partial}{\partial x_2}\cdot\right) + \frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)\right], \tag{2.6h}$$

$$k_{33} = -\mu^{-1}\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right) + \frac{\partial}{\partial x_3}\left((\lambda + 2\mu)\frac{\partial}{\partial x_3}\cdot\right) + \rho\omega^2\right], \tag{2.6i}$$

and

$$l_{11} = -(\lambda + 2\mu)^{-1}\left[\frac{\partial}{\partial x_1}(\lambda + 2\mu)\right], \tag{2.7a}$$

$$l_{12} = -(\lambda + 2\mu)^{-1}\left[\lambda\left(\frac{\partial}{\partial x_2}\cdot\right) + \frac{\partial}{\partial x_2}(\mu\cdot)\right], \tag{2.7b}$$

$$l_{13} = -(\lambda + 2\mu)^{-1}\left[\lambda\left(\frac{\partial}{\partial x_3}\cdot\right) + \frac{\partial}{\partial x_3}(\mu\cdot)\right], \tag{2.7c}$$

$$l_{21} = -\mu^{-1}\left[\frac{\partial}{\partial x_2}(\lambda\cdot) + \mu\left(\frac{\partial}{\partial x_2}\cdot\right)\right], \tag{2.7d}$$

$$l_{22} = -\mu^{-1}\left(\frac{\partial\mu}{\partial x_1}\right), \tag{2.7e}$$

$$l_{23} = l_{32} = 0, \tag{2.7f}$$

$$l_{31} = -\mu^{-1}\left[\frac{\partial}{\partial x_3}(\lambda\cdot) + \mu\left(\frac{\partial}{\partial x_3}\cdot\right)\right], \tag{2.7g}$$

$$l_{33} = -\mu^{-1}\left(\frac{\partial\mu}{\partial x_1}\right). \tag{2.7h}$$

It is convenient to rewrite the system in a 6×6 first-order form as

$$\frac{\partial}{\partial x_1}\begin{pmatrix}\mathbf{u}(\mathbf{r})\\ \mathbf{u}_{,x_1}(\mathbf{r})\end{pmatrix}=B\begin{pmatrix}\mathbf{u}\\ \mathbf{u}_{,x_1}\end{pmatrix}=\begin{pmatrix}\theta & 1\\ K & L\end{pmatrix}\begin{pmatrix}\mathbf{u}\\ \mathbf{u}_{,x_1}\end{pmatrix},\tag{2.8}$$

where θ and 1 are the 3×3 zero and unit matrices. The motivation for rewriting Eq. (2.1) in the form Eq. (2.8) is twofold. First, using $\mathbf{u}$, $\mathbf{u}_{,x_1}$ in the system allows a straightforward transformation to a system of equations involving the $u_j^{\pm}$'s. Secondly, the coefficient matrix is of a form that generates a system which contains only first-order derivatives in x_1 and no mixed derivatives involving x_1.

To define the new wave variables $u_j^{\pm}$, let

$$\mathbf{u}^{+}(\mathbf{r})=\begin{pmatrix}u_1^{+}(\mathbf{r})\\ u_2^{+}(\mathbf{r})\\ u_3^{+}(\mathbf{r})\end{pmatrix}\tag{2.9}$$

and

$$\mathbf{u}^{-}(\mathbf{r})=\begin{pmatrix}u_1^{-}(\mathbf{r})\\ u_2^{-}(\mathbf{r})\\ u_3^{-}(\mathbf{r})\end{pmatrix}\tag{2.10}$$

and set

$$\begin{pmatrix}\mathbf{u}^{+}(\mathbf{r})\\ \mathbf{u}^{-}(\mathbf{r})\end{pmatrix}=S\begin{pmatrix}\mathbf{u}(\mathbf{r})\\ \mathbf{u}_{,x_1}(\mathbf{r})\end{pmatrix},\tag{2.11}$$

where S is the 6×6 *splitting matrix*. The general splitting matrix is given by

$$S=P^{-1}WP,\tag{2.12}$$

where

$$P=\begin{pmatrix}1&0&0&0&0&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&0&0&1&0\\0&0&1&0&0&0\\0&0&0&0&0&1\end{pmatrix}\tag{2.13}$$

and

$$W=\frac{1}{2}\begin{pmatrix}W_1&0&0\\0&W_2&0\\0&0&W_3\end{pmatrix}.\tag{2.14}$$

In Eq. (2.14), "0" is the 2×2 zero matrix and the three 2×2 matrices W_j, $j=1,2,3$, are in the form

$$W_j=\begin{pmatrix}1 & -iw_j(\mathbf{r})^{-1}\\ 1 & iw_j(\mathbf{r})^{-1}\end{pmatrix},\tag{2.15}$$

where the functions $w_j(\mathbf{r})$ are defined below. Each choice of a set of functions $\{w_j;j=1,2,3\}$ specifies a 6×6 matrix W through Eq. (2.14), which defines a corresponding splitting matrix S through Eq. (2.12). The permutation matrix P defined in Eq. (2.12) rearranges the components of $\mathbf{u}$ and $\mathbf{u}_{,x_1}$ making the variables u_j and u_{j,x_1} nearest neighbors, for each j, in the 6×1 column vectors in Eq. (2.8). Each component of the six equations combined in Eq. (2.11) is in the form

$$u_j^{\pm}=\tfrac{1}{2}(u_j\mp iw_j^{-1}u_{j,x_1}).$$

The next step is to derive the equations for the $u_j^{\pm}$. To do this let $\mathbf{U}$ be the 6-vector

$$\mathbf{U}(\mathbf{r})=\begin{pmatrix}\mathbf{u}^{+}(\mathbf{r})\\ \mathbf{u}^{-}(\mathbf{r})\end{pmatrix}\tag{2.16}$$

and rewrite Eq. (2.8) as

$$\begin{aligned}\frac{\partial}{\partial x_1}\mathbf{U}&=\left[\frac{\partial S}{\partial x_1}S^{-1}+SBS^{-1}\right]\mathbf{U}\\ &=\begin{pmatrix}T^{++} & R^{+-}\\ R^{-+} & T^{--}\end{pmatrix}\mathbf{U},\end{aligned}\tag{2.17}$$

where

$$T^{++}=\frac{1}{2}\left(\frac{\partial F}{\partial x_1}F^{-1}-F^{-1}-FK+FL\,F^{-1}\right),\tag{2.18a}$$

$$R^{+-}=\frac{1}{2}\left(-\frac{\partial F}{\partial x_1}F^{-1}+F^{-1}-FK-FL\,F^{-1}\right),\tag{2.18b}$$

$$R^{-+}=\frac{1}{2}\left(-\frac{\partial F}{\partial x_1}F^{-1}-F^{-1}+FK-FL\,F^{-1}\right),\tag{2.18c}$$

and

$$T^{--}=\frac{1}{2}\left(\frac{\partial F}{\partial x_1}F^{-1}+F^{-1}+FK+FL\,F^{-1}\right).\tag{2.18d}$$

In Eqs. (2.18a)–(2.18d), K and L are the 3×3 matrices of Eq. (2.5) and F is the 3×3 matrix

$$F=i\begin{pmatrix}w_1(\mathbf{r})^{-1}&0&0\\0&w_2(\mathbf{r})^{-1}&0\\0&0&w_3(\mathbf{r})^{-1}\end{pmatrix}.\tag{2.19}$$

The block off-diagonal terms R^{+-} and R^{-+} in Eq. (2.17) are interpreted as infinitesimal reflection operators, i.e., operators which couple forward and backward moving waves. It is easy to show that the 3×3 matrices in Eq. (2.18) satisfy the conjugation symmetry relations

$$T^{++}=(t_{ij}),\tag{2.20a}$$

$$R^{+-}=(r_{ij}),\tag{2.20b}$$

$$R^{-+}=(r_{ij}^{*})=[R^{+-}]^{*},\tag{2.20c}$$

$$T^{--}=(t_{ij}^{*})=[T^{++}]^{*},\tag{2.20d}$$

where i and j range over values 1,2,3 independently and the superscript asterisks denote complex conjugations. The elements t_{ij} and r_{ij} are given by the equations

$$\begin{aligned}t_{11}=\frac{1}{2}\Big\{&-\frac{\partial}{\partial x_1}(\ln w_1)+iw_1-\frac{\partial}{\partial x_1}\ln(\lambda+2\mu)\\ &+i\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)\right.\\ &\left.+\rho\omega^2\right]/[(\lambda+2\mu)w_1]\Big\}.\end{aligned}\tag{2.21a}$$

$$\begin{aligned}t_{12}=\frac{1}{2}\Big\{\Big[&i\frac{\partial\lambda}{\partial x_1}\left(\frac{\partial}{\partial x_2}\cdot\right)-\lambda\frac{\partial}{\partial x_2}(w_2\cdot)\\ &-\frac{\partial}{\partial x_2}(\mu w_2\cdot)\Big]/[(\lambda+2\mu)\,w_1]\Big\}.\end{aligned}\tag{2.21b}$$

$$\begin{aligned}t_{13}=\frac{1}{2}\Big\{\Big[&i\frac{\partial\lambda}{\partial x_1}\left(\frac{\partial}{\partial x_3}\cdot\right)-\lambda\frac{\partial}{\partial x_3}(w_3\cdot)\\ &-\frac{\partial}{\partial x_3}(\mu w_3\cdot)\Big]/[(\lambda+2\mu)\,w_1]\Big\}.\end{aligned}\tag{2.21c}$$

$$t_{21}=\frac{1}{2}\left\{\left[i\frac{\partial\mu}{\partial x_1}\left(\frac{\partial}{\partial x_2}\cdot\right)-\mu\frac{\partial}{\partial x_2}(w_2\cdot)\right.\right.$$
$$\left.\left.-\frac{\partial}{\partial x_2}(\lambda w_1\cdot)\right]/[\mu w_2]\right\}, \quad (2.21d)$$

$$t_{22}=\frac{1}{2}\left\{-\frac{\partial}{\partial x_1}(\ln w_2)+iw_2-\frac{\partial}{\partial x_1}(\ln\mu)\right.$$
$$+i\left[\frac{\partial}{\partial x_2}\left((\lambda+2\mu)\frac{\partial}{\partial x_2}\cdot\right)\right.$$
$$\left.\left.+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)+\rho\omega^2\right]/[\mu w_2]\right\}, \quad (2.21e)$$

$$t_{23}=\tfrac{1}{2}i\left\{\left[\frac{\partial}{\partial x_2}\left(\lambda\frac{\partial}{\partial x_3}\cdot\right)+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)\right]/[\mu w_2]\right\}, \quad (2.21f)$$

$$t_{31}=\tfrac{1}{2}\left\{\left[i\frac{\partial\mu}{\partial x_1}\left(\frac{\partial}{\partial x_3}\cdot\right)-\mu\frac{\partial}{\partial x_3}(w_1\cdot)\right.\right.$$
$$\left.\left.-\frac{\partial}{\partial x_3}(\lambda w_1\cdot)\right]/[\mu w_3]\right\}, \quad (2.21g)$$

$$t_{32}=\tfrac{1}{2}i\left\{\left[\frac{\partial}{\partial x_3}\left(\lambda\frac{\partial}{\partial x_2}\cdot\right)+\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)/[\mu w_3]\right]\right\}, \quad (2.21h)$$

$$t_{33}=\tfrac{1}{2}\left\{-\frac{\partial}{\partial x_1}(\ln w_3)+iw_3-\frac{\partial}{\partial x_1}(\ln\mu)\right.$$
$$+i\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)\right.$$
$$\left.\left.+\frac{\partial}{\partial x_3}\left((\lambda+2\mu)\frac{\partial}{\partial x_3}\cdot\right)+\rho\omega^2\right]/[\mu w_3]\right\}, \quad (2.21i)$$

$$r_{11}=\frac{1}{2}\left\{\frac{\partial}{\partial x_1}(\ln w_1)-iw_1+\frac{\partial}{\partial x_1}(\ln(\lambda+2\mu)).\right.$$
$$+i\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)\right.$$
$$\left.\left.+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)+\rho\omega^2\right]/[(\lambda+2\mu)w_1]\right\}, \quad (2.21j)$$

$$r_{12}=-t^*_{12}, \quad (2.21k)$$
$$r_{13}=-t^*_{13}, \quad (2.21l)$$
$$r_{21}=-t^*_{21}, \quad (2.21m)$$

$$r_{22}=\frac{1}{2}\left\{\frac{\partial}{\partial x_1}(\ln w_2)-iw_2+\frac{\partial}{\partial x_1}(\ln\mu)\right.$$
$$+i\left[\frac{\partial}{\partial x_2}\left((\lambda+2\mu)\frac{\partial}{\partial x_2}\cdot\right)\right.$$
$$\left.\left.+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)+\rho\omega^2\right]/[\mu w_2]\right\}, \quad (2.21n)$$

$$r_{23}=t_{23}, \quad (2.21o)$$
$$r_{31}=-t^*_{31}, \quad (2.21p)$$
$$r_{32}=t_{32}, \quad (2.21q)$$

and

$$r_{33}=\frac{1}{2}\left\{\frac{\partial}{\partial x_1}(\ln w_3)-iw_3+\frac{\partial}{\partial x_1}(\ln\mu)\right.$$
$$+i\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)\right. \quad (2.21r)$$
$$\left.\left.+\frac{\partial}{\partial x_3}\left((\lambda+2\mu)\frac{\partial}{\partial x_3}\cdot\right)+\rho\omega^2\right]/[\mu w_3]\right\}.$$

The equations in Eq. (2.17) combined with Eqs. (2.20) and (2.21) are *equivalent* to Eq. (2.1); it is just that in the former the information is expressed in terms of the variables $u_j^\pm$, with a clear physical interpretation.

To arrive at a parabolic approximation it is necessary to specify a set of functions $\{w_j; j=1,2,3\}$. As a first example set

$$w_1=k_L=\left(\frac{\rho\omega^2}{\lambda+2\mu}\right)^{1/2} \quad (2.22a)$$

and

$$w_2=w_3=k_T=\left(\frac{\rho\omega^2}{\mu}\right)^{1/2}. \quad (2.22b)$$

To avoid the unnecessary reproduction of very similar equations, the fast phase terms will now be introduced. The following definitions are required.

$$\rho(\mathbf{r})=\rho_0(1+\tilde\rho(\mathbf{r})), \quad (2.23a)$$
$$\mu(\mathbf{r})=\mu_0(1+\tilde\mu(\mathbf{r})), \quad (2.23b)$$
$$\lambda(\mathbf{r})=\lambda_0(1+\tilde\lambda_0(\mathbf{r})), \quad (2.23c)$$
$$k_{L0}=\left(\frac{\rho_0\omega^2}{\lambda_0+2\mu_0}\right)^{1/2}, \quad (2.24a)$$

and

$$k_{T0}=(\rho_0\omega^2/\mu_0)^{1/2}. \quad (2.24b)$$

With this notation

$$u_1^\pm(\mathbf{r})=v_1^\pm e^{\pm ik_{L0}x_1}, \quad (2.25a)$$
$$u_l^\pm(\mathbf{r})=v_l^\pm e^{\pm ik_{T0}x_1}, \quad (2.25b)$$

for $l=2,3$. The additional notation

$$\mathbf{v}^\pm=\begin{pmatrix}v_1^\pm\\ v_2^\pm\\ v_3^\pm\end{pmatrix} \quad (2.26a)$$

and

$$\mathbf{v}=\begin{pmatrix}\mathbf{v}^+\\ \mathbf{v}^-\end{pmatrix} \quad (2.26b)$$

will be convenient. The equation for $\mathbf{v}$, which follows readily from Eq. (2.17), is

$$\mathbf{v}_{,x_1}=\begin{pmatrix}T_1^{++} & R_1^{+-}\\ R_1^{-+} & T_1^{--}\end{pmatrix}\cdot\mathbf{v}, \quad (2.27a)$$

with

$$T_1^{++}=(t_{1,ij}^{++}). \quad (2.27b)$$

The elements in the matrix on the right-hand side of Eq. (2.27b) are

$$t_{1,11}^{++}=-\frac{1}{4}\frac{\partial}{\partial x_1}(\ln(\rho))-\frac{1}{4}\frac{\partial}{\partial x_1}(\ln(\lambda+2\mu))+i(w_1-k_{L0}$$
$$+i\left[\frac{\partial}{\partial x_2}\left(\mu\frac{\partial}{\partial x_2}\cdot\right)+\frac{\partial}{\partial x_3}\left(\mu\frac{\partial}{\partial x_3}\cdot\right)\right]\Big/[4\rho\omega^2(\lambda+2\mu)]^{1/2} \quad (2.28a)$$

$$t_{1,12}^{++}=\tfrac{1}{2}e^{i(k_{T0}-k_{L0})x_1}\left[i\left(\frac{\partial\lambda}{\partial x_1}\right)\left(\frac{\partial}{\partial x_2}\cdot\right)=\lambda\frac{\partial}{\partial x_2}(w_2\cdot)\right.$$
$$\left.-\frac{\partial}{\partial x_2}(\mu w_2\cdot)\right]/[\rho\omega^2(\lambda+2\mu)]^{1/2}, \quad (2.28b)$$

$$t_{1,13}^{+\ +} = \tfrac{1}{2}\, e^{i(k_{TO} - k_{LO})x_1}\Big[i\Big(\frac{\partial \lambda}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_3}\cdot\Big) + \lambda\frac{\partial}{\partial x_3}(w_3\,\cdot) - \frac{\partial}{\partial x_3}(\mu w_3\,\cdot)\Big]\Big/[\rho\omega^2(\lambda + 2\mu)]^{1/2}, \tag{2.28c}$$

$$t_{1,21}^{+\ +} = \tfrac{1}{2} e^{i(k_{LO} - k_{TO})x_1}\Big[i\Big(\frac{\partial \mu}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_2}\cdot\Big) - \mu\frac{\partial}{\partial x_2}(w_1\,\cdot) - \frac{\partial}{\partial x_2}(\lambda w_1\,\cdot)\Big]\Big/[\rho\omega^2\mu]^{1/2}, \tag{2.28d}$$

$$t_{1,22}^{+\ +} = -\frac{1}{4}\frac{\partial}{\partial x_1}(\ln\rho) - \frac{1}{4}\frac{\partial}{\partial x_1}(\ln\mu) + i(w_2 - k_{TO}) + i\Big[\frac{\partial}{\partial x_3}\Big(\mu\frac{\partial}{\partial x_3}\cdot\Big) + \frac{\partial}{\partial x_2}\Big((\lambda + 2\mu)\frac{\partial}{\partial x_2}\cdot\Big)\Big]\Big/[4\rho\omega^2\mu]^{1/2}, \tag{2.28e}$$

$$t_{1,23}^{+\ +} = \frac{1}{2}i\Big[\frac{\partial}{\partial x_2}\Big(\lambda\frac{\partial}{\partial x_3}\cdot\Big) + \frac{\partial}{\partial x_3}\Big(\mu\frac{\partial}{\partial x_2}\cdot\Big)\Big]\Big/[\rho\omega^2\mu]^{1/2}, \tag{2.28f}$$

$$t_{1,31}^{+\ +} = \tfrac{1}{2} e^{i(k_{LO} - k_{TO})x_1}\Big[i\Big(\frac{\partial \mu}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_3}\cdot\Big) - \mu\frac{\partial}{\partial x_3}(w_1\,\cdot) - \frac{\partial}{\partial x_3}(\lambda w_1\,\cdot)\Big]\Big/[\rho\omega^2\mu]^{1/2}, \tag{2.28g}$$

$$t_{1,32}^{+\ +} = \tfrac{1}{2}i\Big[\frac{\partial}{\partial x_3}\Big(\lambda\frac{\partial}{\partial x_2}\cdot\Big) + \frac{\partial}{\partial x_2}\Big(\mu\frac{\partial}{\partial x_3}\cdot\Big)\Big]\Big/[\rho\omega^2\mu]^{1/2}, \tag{2.28h}$$

and

$$t_{1,33}^{+\ +} = -\frac{1}{4}\frac{\partial}{\partial x_1}(\ln\rho) - \frac{1}{4}\frac{\partial}{\partial x_1}(\ln\mu) + i(w_3 - k_{TO}) + i\Big[\frac{\partial}{\partial x_2}\Big(\mu\frac{\partial}{\partial x_2}\cdot\Big) + \frac{\partial}{\partial x_3}\Big((\lambda + 2\mu)\frac{\partial}{\partial x_3}\cdot\Big)\Big]\Big/[4\rho\omega^2\mu]^{1/2}. \tag{2.28i}$$

The reflection matrix elements

$$R_1^{+\ -} = (r_1^{+\ -}) \tag{2.29a}$$

are given by

$$r_{1,11}^{+\ -} = r_{11}^{+\ -} e^{-2ik_{LO}x_1}, \tag{2.29b}$$

$$r_{1,12}^{+\ -} = r_{12}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29c}$$

$$r_{1,13}^{+\ -} = r_{13}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29d}$$

$$r_{1,21}^{+\ -} = r_{21}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29e}$$

$$r_{1,22}^{+\ -} = r_{22}^{+\ -} e^{-2ik_{LO}x_1}, \tag{2.29f}$$

$$r_{1,23}^{+\ -} = r_{23}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29g}$$

$$r_{1,31}^{+\ -} = r_{31}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29h}$$

$$r_{1,32}^{+\ -} = r_{32}^{+\ -} e^{-i(k_{LO} + k_{TO})x_1}, \tag{2.29i}$$

and

$$r_{1,33}^{+\ -} = r_{33}^{+\ -} e^{-2ik_{LO}x_1}. \tag{2.29j}$$

Similar expressions for $T_1^{-\ -}$ and $R_1^{-\ +}$ can be obtained.

It is interesting to note that the phases in Eqs. (2.28) and (2.29) are just those obtained from wave-number (momentum) conservation. As an example, consider the transition from a downward-moving longitudinal wave u_1^- to an upward-moving transverse wave u_2^+. The reflection matrix element involved $r_{1,21}^{+\ -}$ and has the phase $i(k_{LO} + k_{TO})x_1$, which is similar to the scalar case.

The parabolic approximation to Eq. (2.27) is obtained by suppressing the reflection terms. This is valid when the functions $\{\tilde\rho,\tilde\mu,\tilde\lambda\}$ in Eq. (2.23) are small compared to 1 and are slowly varying in (x_1,x_2,x_3) on the length scale of the carrier waves. In this case, the phases of all terms in $R_1^{+\ -}$ and $R_1^{-\ +}$ vary rapidly making these terms negligible in the lowest order approximation. Thus, the parabolic approximation for $\mathbf{v}^+$ is given by

$$\frac{\partial}{\partial x_1}(\mathbf{v}^+) = T_1^{+\ +}\cdot\mathbf{v}_1^+ \tag{2.30a}$$

and the approximation for $\mathbf{v}^-$ is given by

$$\frac{\partial}{\partial x_1}(\mathbf{v}^-) = T_1^{-\ -}\cdot\mathbf{v}^-. \tag{2.30b}$$

Clearly other choices of splitting, i.e., the w_j's, yield different parabolic approximations. Likewise various physical assumptions may make it useful to assume wave numbers for carrier waves different from that in Eq. (2.25). This case is described in Sec. 5, where a comparison is made with a parabolic approximation by Hudson.[9]

A second natural splitting is completely parallel to both the scalar- and the Fock-parabolic approximation to the Helmholtz equation.[5] This splitting is defined by

$$w_1 = k_{LO} \tag{2.31a}$$

and

$$w_2 = w_3 = k_{TO}. \tag{2.31b}$$

In a slight abuse of notation, the approximate upward- and downward-moving waves are again denoted as $u_j^\pm$ and again the amplitudes and phases are chosen such that Eq. (2.25) holds. Using the same reasoning as before it follows that this leads to a new parabolic approximation

$$\frac{\partial}{\partial x_1}(\mathbf{v}^+) = T_0^{+\ +}\cdot\mathbf{v}^+, \tag{2.32a}$$

where

$$T_0^{+\ +} = (t_{0,ij}^{+\ +}). \tag{2.32b}$$

The matrix elements of Eq. (2.32b) are

$$t_{0,11}^{+\ +} = \tfrac{1}{2}\Big[-iw_1^2(\lambda + 2\mu) - w_1\frac{\partial}{\partial x_1}(\lambda + 2\mu) + i\rho\omega^2 + i\frac{\partial}{\partial x_2}\Big(\mu\frac{\partial}{\partial x_2}\cdot\Big) + i\frac{\partial}{\partial x_3}\Big(\mu\frac{\partial}{\partial x_3}\cdot\Big)\Big/[w_1(\lambda + 2\mu)], \tag{2.33a}$$

$$t_{0,12}^{+\ +} = \tfrac{1}{2} e^{i(k_{TO} - k_{LO})x_1}\Big[i\Big(\frac{\partial\lambda}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_2}\cdot\Big) - \lambda w_2\Big(\frac{\partial}{\partial x_2}\cdot\Big) - w_2\frac{\partial}{\partial x_2}(\mu\cdot)\Big]\Big/[w_1(\lambda + 2\mu)], \tag{2.33b}$$

$$t_{0,13}^{+\ +} = \tfrac{1}{2} e^{i(k_{TO} - k_{LO})x_1}\Big[i\frac{\partial\lambda}{\partial x_1}\Big(\frac{\partial}{\partial x_3}\cdot\Big) - \lambda w_3\Big(\frac{\partial}{\partial x_3}\cdot\Big) - w_3\frac{\partial}{\partial x_3}(\mu\cdot)\Big]\Big/[w_1(\lambda + 2\mu)], \tag{2.33c}$$

$$t_{0,21}^{+\ +} = \tfrac{1}{2} e^{i(k_{LO} - k_{TO})x_1}\Big[i\Big(\frac{\partial\mu}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_2}\cdot\Big) - \mu w_2\Big(\frac{\partial}{\partial x_2}\cdot\Big)$$

$$- w_1 \frac{\partial}{\partial x_2} (\lambda \cdot) \Big] / [w_2 \mu], \tag{2.33d}$$

$$t^{+}_{0,22}{}^{+} = \tfrac{1}{2}\Big[- i w_2^2 \mu - w_2 \Big(\frac{\partial \mu}{\partial x_1}\Big) + i\rho\omega^2 + i \frac{\partial}{\partial x_3}\Big(\mu \frac{\partial}{\partial x_3}\cdot\Big) + i \frac{\partial}{\partial x_2}\Big((\lambda + 2\mu)\frac{\partial}{\partial x_2}\cdot\Big)\Big] / [w_2 \mu], \tag{2.33e}$$

$$t^{+}_{0,23}{}^{+} = \tfrac{1}{2} i\Big[\frac{\partial}{\partial x_2}\Big(\lambda \frac{\partial}{\partial x_3}\cdot\Big) + \frac{\partial}{\partial x_3}\Big(\mu \frac{\partial}{\partial x_2}\cdot\Big)\Big] / [w_2 \mu], \tag{2.33f}$$

$$t^{+}_{0,31}{}^{+} = \tfrac{1}{2} e^{i(k_{L,0} - k_{T0})x_1}\Big[i \Big(\frac{\partial \mu}{\partial x_1}\Big)\Big(\frac{\partial}{\partial x_3}\cdot\Big) - \mu w_1 \Big(\frac{\partial}{\partial x_3}\cdot\Big) - w_1 \frac{\partial}{\partial x_3}(\lambda\cdot)\Big] / [w_3 \mu], \tag{2.33g}$$

$$t^{+}_{0,32}{}^{+} = \tfrac{1}{2} i\Big[\frac{\partial}{\partial x_3}\Big(\lambda \frac{\partial}{\partial x_2}\cdot\Big) + \frac{\partial}{\partial x_2}\Big(\mu \frac{\partial}{\partial x_3}\cdot\Big)\Big] / [w_3 \mu], \tag{2.33h}$$

and

$$t^{+}_{0,33}{}^{+} = \tfrac{1}{2}\Big[- i w_3^2 \mu - w_3 \Big(\frac{\partial \mu}{\partial x_1}\Big) + i\rho\omega^2 + i \frac{\partial}{\partial x_2}\Big(\mu \frac{\partial}{\partial x_2}\cdot\Big) + i \frac{\partial}{\partial x_3}\Big((\lambda + 2\mu)\frac{\partial}{\partial x_3}\cdot\Big)\Big] / [w_3 \mu]. \tag{2.33i}$$

This completes the derivation of two parabolic approximations to Eq. (2.1). In the next section some heuristic arguments are presented which strongly suggest that the interpretation of the $u_j^{\pm}$'s, especially as associated with Eq. (2.22), is indeed correct for elastic media with small, slowly varying inhomogeneities.

3. HEURISTICS OF THE SPLITTING SCHEME

As mentioned in Sec. 2, the functions $u_j^{\pm}(\mathbf{r}), j = 1,2,3$, can be interpreted physically provided that a reasonable splitting scheme is used. To justify this heuristically, both the scalar wave equation and the reflection–refraction properties of an elastic wave at the interface between two homogeneous media will be shown to suggest the same splitting scheme.

Looking first at the scalar wave equation in one dimension,

$$\frac{d^2\psi}{dx^2} + k^2(x)\psi(x) = 0, \tag{3.1}$$

it is well known[1,4,5] that the splitting

$$\begin{pmatrix}\psi^+(x)\\ \psi^-(x)\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -ik(x)^{-1}\\ 1 & ik(x)^{-1}\end{pmatrix}\begin{pmatrix}\psi(x)\\ (d\psi/dx)(x)\end{pmatrix} \tag{3.2}$$

yields a "parabolic" approximation for the functions ψ^+ and ψ^-. It has been known since the work of Bremmer[1] that these functions are the "forward" and "backward" moving components of ψ, respectively. If

$$k^2(x) = k_0^2(1 + \eta(x)) \tag{3.3}$$

with $\eta(x)$ small and slowly varying, a second splitting scheme can be written as

$$\begin{pmatrix}\psi_0^+(x)\\ \psi_0^-(x)\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & -ik_0^{-1}\\ 1 & ik_0^{-1}\end{pmatrix}\begin{pmatrix}\psi(x)\\ (d\psi/dx)(x)\end{pmatrix}. \tag{3.4}$$

This scheme is, in general, computationally more convenient than that in Eq. (3.2) but the functions $\psi_0^{\pm}$ are approximations to $\psi^{\pm}$.

The three-dimensional scalar wave equation

$$\Delta\psi(\mathbf{r}) + \mathrm{k}^2(\mathbf{r})\,\psi(\mathbf{r}) = 0 \tag{3.5}$$

has similar splitting schemes.[5] It is assumed that there is a preferred direction of propagation, say x_1, and in this case the term $d\psi/dx$ in Eqs. (3.2) and (3.4) is replaced by $\partial\psi/\partial x_1$. The functions $\psi^{\pm}$ are then the components of ψ moving in the $\pm x_1$ direction and $\psi_0^{\pm}$ are approximations to $\psi^{\pm}$.

The splitting schemes used in Sec. 2 are analogous to Eqs. (3.2) and (3.4). From Eqs. (2.11)–(2.15) it is seen that

$$\begin{pmatrix}u_j^+\\ u_j^-\end{pmatrix} = \frac{1}{2} W_j \begin{pmatrix}u_j\\ \partial u_j/\partial x_1\end{pmatrix} \tag{3.6}$$

for $j = 1,2,3$. Thus, it is reasonable to assume upon using Eqs. (2.23a)–(2.23c) that $u_1^{\pm}$ are the components of a longitudinal wave moving in the $\pm x_1$ direction. Similarly, $u_2^{\pm}$ and $u_3^{\pm}$ are the components of transverse waves moving in the $\pm x_1$ direction.

This interpretation of the $u_j^{\pm}$'s is supported by comparison of the parabolic approximation Eqs. (2.30a) and (2.32a) to "infinitesimal transmission and reflection coefficients" obtained from reflection–refraction from a plane interface between two different homogeneous media. In order to display this comparison, consider the configuration shown in Fig. 1. The incident, reflected, and refracted shear waves in Fig. 1 are given by

$$u_{\text{inc},s} = A e^{ik'_T(x_2 \sin\theta_0 + x_1\cos\theta_0)}, \tag{3.7}$$

$$u_{\text{refl},s} = B e^{ik'_T(x_2 \sin\theta_0 - x_1\cos\theta_0)}, \tag{3.8}$$

and

$$u_{\text{refr},s} = A' e^{ik''_T(x_2 \sin\theta_1 + x_1\cos\theta_1)}, \tag{3.9}$$

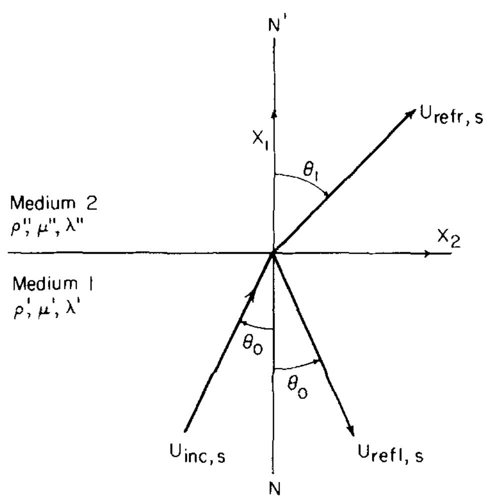

FIG. 1. Geometry for a shear wave incident at the plane interface between two homogeneous media. Medium 1 has constitutive parameters (ρ', μ', λ') and medium 2 has constitutive parameters $(\rho'', \mu'', \lambda'')$. The angle of incidence is θ_0, the angle of reflection is also θ_0, the angle of refraction is θ_1, and all angles are measured from NN', the normal to the interface. The x_1-coordinate axis lies along the normal NN' and the x_2-coordinate axis is in the plane of the interface between the media. All waves are transverse or shear waves.

where

$$k'_T = (\rho'\omega^2/\mu')^{1/2} \qquad (3.10a)$$

and

$$k''_T = (\rho''\omega^2/\mu'')^{1/2}. \qquad (3.10b)$$

Using the continuity of the displacement and stress at the interface, on p. 184 of Ref. 12, it is shown that

$$A' = \frac{2\mu'\cos\theta_0}{[\mu'\cos\theta_0 + \mu''(k''_T/k'_T)\cos\theta_1]} A_0 \qquad (3.11)$$

and

$$B = \frac{[\mu'\cos\theta_0 - \mu''(k''_T/k'_T)\cos\theta_0]}{[\mu'\cos\theta_0 + \mu''(k''_T/k'_T)\cos\theta_1]} A_0. \qquad (3.12)$$

Define μ' and μ'' by

$$\mu' = \mu(-\Delta x_1/2, 0, 0), \qquad (3.13a)$$

$$\mu'' = \mu(\Delta x_1/2, 0, 0), \qquad (3.13b)$$

where the function μ is the transverse Lamé parameter of Sec. 2. Assume similar definitions for ρ', ρ'', λ', and λ''. Then to first order

$$\mu'' = \mu' + \mu_{,x_1}(-\Delta x_1/2, 0, 0)\Delta x_1, \qquad (3.14a)$$

$$\rho'' = \rho' + \rho_{,x_1}(-\Delta x_1/2, 0, 0)\Delta x_1, \qquad (3.14b)$$

$$\lambda'' = \lambda' + \lambda_{,x_1}(-\Delta x_1/2, 0, 0)\Delta x_1, \qquad (3.14c)$$

and

$$\cos\theta_1 = [1 + c_-\tan^2\theta_0\,\Delta x_1]\cos\theta_0, \qquad (3.14d)$$

where

$$c_\pm = \tfrac{1}{2}[\rho_{,x_1}(-\Delta x_1/2, 0, 0)/\rho' \pm \mu_{,x_1}(-\Delta x_1/2, 0, 0)/\mu']. \qquad (3.14e)$$

It follows that

$$A' = A[1 - \tfrac{1}{2}\{c_-\tan^2\theta_0 + c_+\}\Delta x_1] \qquad (3.15a)$$

and

$$B = -\tfrac{1}{2}Ac_-\tan^2\theta_0\,\Delta x_1. \qquad (3.15b)$$

Consistent with the parabolic approximation, assume that θ_0 is small so that

$$\cos\theta_0 \approx 1,$$

$$\sin\theta_0 \approx \theta_0,$$

$$\tan^2\theta_0 \approx 0.$$

Then the rate of change of the forward moving component of the shear wave is

$$\lim_{\Delta x_1 \to 0} \left\{\frac{u_{\text{refr},s} - u_{\text{inc},s}}{\Delta x_1}\right\} = \left\{-\frac{1}{4}\left[\frac{\rho_{,x_1}}{\rho} + \frac{\mu_{,x_1}}{\mu}\right] + i\left(\frac{\rho\omega^2}{\mu}\right)^{1/2}\right\}\Bigg|_{(0,0,0)} u_{\text{inc},s}\Big|_{(0,0,0)} \qquad (3.16)$$

Identifying $u_{\text{inc},s}$ with u_2^+, the left-hand side of Eq. (3.16) is seen to be $\partial u_2^+/\partial x_1$. Comparing Eq. (3.16) to Eq. (2.27) and allowing for the removal of the fast phase, the right-hand side of Eq. (3.16) clearly agrees with those terms in $t^{+}_{1,22}{}^{+}$ which do not involve transverse derivatives. Furthermore, if $u_{\text{refl},s}$ is identified with u_2^- then Eq. (3.15b) shows that the infinitesimal reflection coefficient is of order $\theta_0^2\,\Delta x_1$. This justifies neglecting reflection terms in the first approximation.

A similar analysis can be performed for a longitudinal wave incident upon a plane interface between two homogeneous media as shown in Fig. 2. The incident, reflected, and refracted longitudinal waves are given by

$$u_{\text{inc},p} = Ae^{ik'_L(x_2\sin\theta_0 + x_1\cos\theta_0)}, \qquad (3.17a)$$

$$u_{\text{refl},p} = Be^{ik'_L(x_2\sin\theta_0 - x_1\cos\theta_0)}, \qquad (3.17b)$$

and

$$u_{\text{refr},p} = A'e^{ik''_L(x_2\sin\theta 2 + x_1\cos\theta_2)}, \qquad (3.17c)$$

where

$$k'_L = \left[\frac{\rho'\omega^2}{(\lambda' + 2\mu')}\right]^{1/2} \qquad (3.17d)$$

and

$$k''_L = \left[\frac{\rho''\omega^2}{(\lambda'' + 2\mu'')}\right]^{1/2}. \qquad (3.17e)$$

The reflected and refracted transverse waves are given by

$$u_{\text{refl},s} = C\,e^{ik'_T(x_2\sin\theta_1 - x_1\cos\theta_1)}, \qquad (3.18a)$$

and

$$u_{\text{refr},s} = C'\,e^{ik''_T(x_2\sin\theta_3 + x_1\cos\theta_3)}, \qquad (3.18b)$$

where k'_T and k''_T are given in Eq. (3.10). Define $\rho', \rho'', \mu', \mu'', \lambda'$, and λ'' as in the previous example and assume that θ_0 is small. Using continuity of the displacement and stress at the interface, it follows from p. 186 of Ref. 12 that to first order

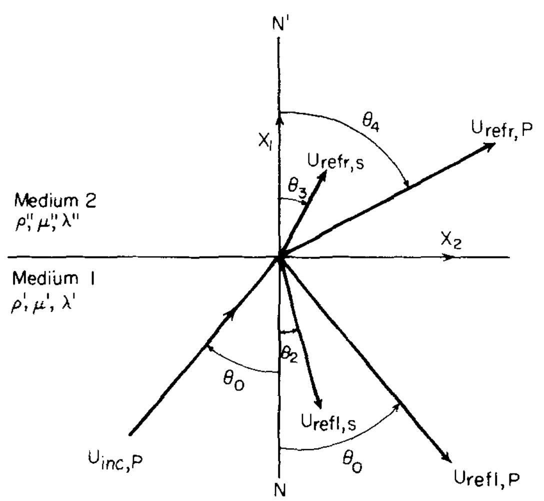

FIG. 2. Geometry for a longitudinal wave incident at the plane interface between two homogeneous media. Medium 1 has constitutive parameters (ρ',μ',λ') and medium 2 has constitutive parameters (ρ'',μ'',λ''). The angle of the incidence is θ_0, the angle of the reflected P wave is θ_0, the angle of the reflected S wave is θ_1, the angle of the refracted P wave is θ_2, and the angle of the refracted S wave is θ_3. All angles are measured from the normal NN'.

$$
\begin{pmatrix} -\theta_0 & 1 & \theta_0(1+\alpha\Delta x_1) & 1 \\ 1 & -\theta_0/\kappa & 1 & \theta_0(1+\beta\Delta x_1)/\kappa \\ 2\theta_0 & \kappa & 2\theta_0(1+\gamma\Delta x_1) & -\kappa[1+(\gamma-\beta)\Delta x_1] \\ -\kappa^2 & 2\theta_0 & \kappa^2[1+(\alpha-2\beta+\gamma)\Delta x_1] & 2\theta_0(1+\gamma\Delta x_1) \end{pmatrix} \begin{pmatrix} B \\ C \\ A' \\ C' \end{pmatrix} = A \begin{pmatrix} \theta_0 \\ 1 \\ 2\theta_0 \\ 2 \end{pmatrix}, \tag{3.19}
$$

where

$$
\alpha = \frac{1}{2}\left[\frac{(\lambda+2\mu)_{,x_1}}{(\lambda+2\mu)} - \frac{\rho_{,x_1}}{\rho}\right]\Bigg|_{(0,0,0)}, \tag{3.20a}
$$

$$
\beta = \frac{1}{2}\left[\frac{\mu_{,x_1}}{\mu} - \frac{\rho_{,x_1}}{\rho}\right]\Bigg|_{(0,0,0)}, \tag{3.20b}
$$

$$
\gamma = \left[\frac{\mu_{,x_1}}{\mu}\right]\Bigg|_{(0,0,0)}, \tag{3.20c}
$$

and

$$
\kappa = \left[\frac{\lambda+2\mu}{\mu}\right]^{1/2}\Bigg|_{(0,0,0)}. \tag{3.20d}
$$

Solving for B, C, A', and C' requires a tedious calculation which gives

$$
A' = A\left[1 - \frac{1}{4}\left\{\frac{\rho_{,x_1}}{\rho} + \frac{(\lambda+2\mu)_{,x_1}}{\lambda+2\mu}\right\}\Bigg|_{(0,0,0)} \Delta x_1\right], \tag{3.21}
$$

while B, C, and C' are all of order $\theta_0 \Delta x_1$. Upon setting

$$
u_{\mathrm{inc},p} = u_1^+ \tag{3.22a}
$$

and

$$
\lim_{\Delta x_1 \to 0} \left\{\frac{u_{\mathrm{refr},p} - u_{\mathrm{inc},p}}{\Delta x_1}\right\} = \frac{\partial u_1^+}{\partial x_1}, \tag{3.22b}
$$

it is apparent that Eq. (3.22a) is equal to the terms in $t^{+}_{1,11}{}^{+}$ which do not contain transverse derivatives.

4. BREMMER SERIES AND PARABOLIC APPROXIMATIONS

Now an integral equation equivalent to Eq. (2.17), including the natural boundary conditions associated with the physical interpretation of the $u_j^\pm$'s, will be derived. Iteration of this equation will provide corrections to the parabolic approximation.

Using Eq. (2.17), define the parabolic operators $P^{\pm}$ by

$$
P^{\pm} = \left[\frac{\partial}{\partial x_1} - T^{\pm\,\pm}\right]. \tag{4.1}
$$

The parabolic approximations are written as

$$
P^+ \mathbf{u}^+ = \mathbf{0} \tag{4.2a}
$$

and

$$
P^- \mathbf{u}^- = \mathbf{0}. \tag{4.2b}
$$

The system of Eq. (2.17) can be expressed as

$$
P^+ \mathbf{u}^+ = R^{+\,-} \mathbf{u}^- \tag{4.3a}
$$

and

$$
P^- \mathbf{u}^- = R^{-\,+} \mathbf{u}^+. \tag{4.3b}
$$

The methods of this work are applicable to the generic problem of finding a solution to Eq. (2.1) with upward-moving waves specified by $\mathbf{W}^+(x_1', x_2, x_3)$ at $x_1 = x_1'$ and downward-moving waves specified $\mathbf{W}^-(x_1'', x_2, x_3)$ at $x_1 = x_1''$, $x_1'' > x_1'$. To apply the form of solution of Eq. (4.2) to Eq. (2.1) four solutions to Eq. (4.2) are needed:

(1) The solution $\mathbf{u}_0^+$ of Eq. (4.2a) such that

$$
\mathbf{u}_0^+(x_1', x_2, x_3) = \mathbf{W}^+(x_1', x_2, x_3).
$$

(2) The matrix solution $G_0^+(\mathbf{r}|\mathbf{r}')$ of Eq. (4.2a) such that

$$
G_0^+(x_1', x_2', x_3', | x_1', x_2'', x_3'') = \delta(x_2' - x_2'')\delta(x_3', -x_3'')1
$$

and

$$
G_0^+(\mathbf{r}|\mathbf{r}') = 0
$$

for all $x_1' > x_1$.

(3) The solution $\mathbf{u}_0^-$ of Eq. (4.2b) such that

$$
\mathbf{u}_0^-(x_1'', x_2, x_3) = \mathbf{W}^-(x_1'', x_2, x_3).
$$

(4) The matrix solution $G_0^-(\mathbf{r}|\mathbf{r}')$ of Eq. (4.2b) such that

$$
G_0^-(x_1', x_2', x_3' | x_1', x_2'', x_3'') = \delta(x_2' - x_2'')\delta(x_3' - x_3'')1
$$

and

$$
G_0^-(\mathbf{r}|\mathbf{r}') = 0
$$

for all $x_1' < x_1$.

With these solutions, Eq. (4.3) can be written as

$$
\mathbf{u}^+(\mathbf{r}) = \mathbf{u}_0^+(\mathbf{r}) + \int_{x_1'}^{x_1} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G_0^+(\mathbf{r}|\mathbf{r}') R^{+\,-}(\mathbf{r}')\mathbf{u}^-(\mathbf{r}')\, d^3\mathbf{r}' \tag{4.4a}
$$

and

$$
\mathbf{u}^-(\mathbf{r}) = \mathbf{u}_0^-(\mathbf{r}) - \int_{x_1}^{x_1''} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G_0^-(\mathbf{r}|\mathbf{r}') R^{-\,+}(\mathbf{r}')\mathbf{u}^+(\mathbf{r}')\, d^3\mathbf{r}'. \tag{4.4b}
$$

The boundary conditions are satisfied by Eq. (4.4) and by explicit differentiation it is easy to show that Eq. (4.4) satisfies Eq. (4.3). If Eq. (4.4) converges, iteration of it yields a series solution with a clear physical interpretation. The zeroth order solution consists of two uncoupled waves, one moving upward and one moving downward along the x_1 axis. The first order solution adds a term that converts upward to downward waves (and vice versa). The next order solution adds all double reflections, and so on. The first iteration is of particular interest since it yields the lowest order approximation for reflected waves—a problem of considerable interest in geophysical applications. This series solution is the Bremmer series for the elastic wave equation.[5]

It is interesting to note that a different system of integral equations can be obtained by using just the diagonal terms of Eq.(2.17). Set

$$P_j^+ = \frac{\partial}{\partial x_1} - t_{jj} \tag{4.5a}$$

and

$$P_j^- = \frac{\partial}{\partial x_1} - t_{jj}^* \tag{4.5b}$$

for $j = 1, 2, 3$ and let

$$P_0^\pm = \begin{pmatrix} P_1^\pm & 0 & 0 \\ 0 & P_2^\pm & 0 \\ 0 & 0 & P_3^\pm \end{pmatrix}. \tag{4.6}$$

Then an extremely crude approximation to Eq. (2.17) is given by

$$P_0^+ \mathbf{u}^+ = \mathbf{0}, \tag{4.7a}$$

$$P_0^- \mathbf{u}^- = \mathbf{0}. \tag{4.7b}$$

In this approximation, coupling between longitudinal and transverse components is ignored. The full system of Eq. (2.17) is equivalent to

$$\begin{pmatrix} P_0^+ & 0 \\ 0 & P_0^- \end{pmatrix}\begin{pmatrix} \mathbf{u}^+ \\ \mathbf{u}^- \end{pmatrix} = M\begin{pmatrix} \mathbf{u}^+ \\ \mathbf{u}^- \end{pmatrix}, \tag{4.8}$$

where

$$M = \begin{pmatrix} T^{++} & R^{+-} \\ R^{-+} & T^{--} \end{pmatrix} - \begin{pmatrix} T_D^{++} & 0 \\ 0 & T_D^{--} \end{pmatrix} \tag{4.9}$$

and

$$T_D^{++} = [T_D^{--}]^* = \begin{pmatrix} t_{11} & 0 & 0 \\ 0 & t_{22} & 0 \\ 0 & 0 & t_{33} \end{pmatrix}. \tag{4.10}$$

Now the following functions are needed.

(1) The solution $\mathbf{u}_0^+$ of Eq. (4.7a) such that

$$\mathbf{u}_0^+(x_1', x_2, x_3) = \mathbf{W}^+(x_1', x_2, x_3);$$

(2) the solution $\mathbf{u}_0^-$ of Eq. (4.7b) such that

$$u_0^-(x_1'', x_2, x_3) = \mathbf{W}^-(x_1'', x_2, x_3);$$

(3) the six scalar Green's distributions $G_j^\pm$ for $j = 1,2,3$, which are solutions of

$$P_j^\pm G_j^\pm = 0,$$

taking upper or lower signs throughout, and where

$$G_j^\pm(x_1', x_2', x_3' | x_1'', x_2'', x_3'') = \delta(x_2' - x_2'')\delta(x_3' - x_3''),$$

$$G_j^+(\mathbf{r}|\mathbf{r}') = 0, \quad \text{for } x_1 < x_1',$$

$$G_j^-(\mathbf{r}|\mathbf{r}') = 0, \quad \text{for } x_1 > x_1'.$$

Form the matrices

$$G_D^\pm(\mathbf{r}|\mathbf{r}') = \begin{pmatrix} G_1^\pm(\mathbf{r}|\mathbf{r}') & 0 & 0 \\ 0 & G_2^\pm(\mathbf{r}|\mathbf{r}') & 0 \\ 0 & 0 & G_3^\pm(\mathbf{r}|\mathbf{r}') \end{pmatrix}, \tag{4.11}$$

again taking the upper or lower signs throughout. It follows that the solution to Eq. (4.8) can be written as

$$\mathbf{u}^+(\mathbf{r}) = \mathbf{u}^0(\mathbf{r}) + \int_{x_1'}^{x_1}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G_D^+(\mathbf{r}|\mathbf{r}') \times [(T^{++} - T_D^{++})\mathbf{u}^+(\mathbf{r}') + R^{+-}\mathbf{u}^-(\mathbf{r}')]\, d^3\mathbf{r}' \tag{4.12a}$$

and

$$\mathbf{u}^-(\mathbf{r}) = \mathbf{u}_0^-(\mathbf{r}) - \int_{x_1}^{x_1''}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G_D^-(\mathbf{r}|\mathbf{r}') \times [(T^{--} - T_D^{--})\mathbf{u}^-(\mathbf{r}') + R^{-+}\mathbf{u}^+(\mathbf{r}')]\, d^3\mathbf{r}'. \tag{4.12b}$$

In this case, coupling between longitudinal and transverse components is initially encountered in the first-order solutions, as is coupling between forward and backward moving waves. On the other hand, the scalar Green's distributions in Eq. (4.12a) will generally be easier to compute than the matrix Green's distributions of Eqs. (4.4a) and (4.4b).

5. DISCUSSION AND CONCLUSIONS

The parabolic approximation to the scalar (acoustic) Helmholtz equation is the subject of an extensive literature. A large fraction of this literature is concerned with computer studies of acoustic waves in media with complicated inhomogeneity. Significant advantages accrue to the parabolic approximation for two reasons.

(1) In comparison to the full wave equation, it is relatively simple to integrate.

(2) As opposed to ray or diffraction theory, it is a full wave theory. Thus, a parabolic approximation for the full elastic wave equation in isotropic, inhomogeneous, three-dimensional media should be useful for both geophysical models and for the quantative nondestructive evaluation using ultrasonics.

The available literature on parabolic approximations to the three-dimensional elastic wave equation is surprisingly rare.[9,10] In Ref. 10 a parabolic approximation is derived for stress-wave propagation in linearly inhomogeneous solids. The principal equation derived, Eq. (42) there, is a complicated differential equation involving a spectral average over wave number using a sin*c* function weight. The equation includes mode-conversion and a detailed discussion of the conditions under which the derivation is valid. The disturbance is assumed to be "almost plane-wave" potentials of S type (shear) and P type (compression). The method used to describe these potentials involves four waves together with a constraint relation which reduces the system to its three independent components. The combination of the constraint and the wave number filtering make the resulting parabolic approximations somewhat complicated.

The results in Ref. 9 are simpler than those in Ref. 10 and are more closely related to the present work. The author considers an inhomogeneous medium with two specific types of propagation:

(1) propagation of nearly compressional waves, and
(2) propagation of nearly shear waves.

In each case a particular scaling argument and asymptotic expansion is used. The principal results are Eqs. (13a)–(13c) and (18a) and (18b) of Ref. 9. To use the splitting methods developed here to reproduce those results, the following are needed. For (1) choose the functions

$$w_1 = w_2 = w_3 = k_{\mathrm{LO}}, \tag{5.1}$$

for use in Eq. (2.15), whereas for (2) choose

$$w_1 = w_2 = w_3 = k_{\mathrm{TO}}. \tag{5.2}$$

If in addition to Eq. (5.1), all terms of the form

$$\left(\frac{\partial \lambda}{\partial x_1}\right)\left(\frac{\partial v_2^+}{\partial x_2}\right) \tag{5.3a}$$

and

$$\left(\frac{\partial \lambda}{\partial x_1}\right)\left(\frac{\partial v_3^+}{\partial x_3}\right) \tag{5.3b}$$

are neglected in Eq. (2.30a) then Eq. (13a) of Ref. 9 is obtained. The additional neglect of all second derivatives and all terms of the form

$$\frac{\partial}{\partial x_1}\,[\mu^{1/2} v_2^+] \tag{5.4a}$$

and

$$\frac{\partial}{\partial x_1}\,[\mu^{1/2} v_3^+]\,, \tag{5.4b}$$

together with Eqs. (5.3a) and (5.3b) and (5.1), yields Eqs. (13b) and (13c) of Ref. 9. Similarly, starting from Eq. (5.2) and neglecting all terms of the form in Eqs. (5.3a), (5.3b), and (5.4a), (5.4b) in Eq. (2.17) yields Eqs. (18b) and (18c) of Ref. 9.

One aspect of the approximation derived in Ref. 9 is clarified by comparing Eqs. (5.1) and (5.2) and Eqs. (2.31a) and (2.13b). Since it is not possible for the longitudinal and transverse wave numbers to be equal, it appears that the "amplitude factors" u_j, $j = 1,2,3$, in Ref. 9 contain a considerable amount of phase information. If so, this could violate the assumptions in Ref. 9 concerning the order of magnitude of terms such as $\partial u_1/\partial x_2$.

The parabolic approximations derived in this paper are all based upon splitting methods. The results are simpler than those in Ref. 10, and involve various corrections to Ref. 9 while retaining much of the simplicity of that work. Part of the increased generality of this work over Ref. 9 is due to the fact that both amplitude and phase information are used in two stages of approximation as was also done in Ref. 10. The results obtained here constitute a method to study parabolic approximations rather than one final version. It is important to realize this, since the main test of parabolic approximations resides in numerical simulation of wave propagation. The rich variety of possible inhomogeneities suggests that this general structure should prove valuable. Such questions as numerical stability and rate of convergence, the size of the cone of validity, and which splitting matrices are most efficient in simulating specific classes of inhomogeneity are left to future work.

It should be noted, however, that the Fock parabolic approximation to the Helmholtz equation is derived using a constant splitting matrix.[5] In the elastic wave case the analogous matrix is given by Eqs. (2.31a) and (2.31b). This splitting yields the simplest approximation to Eq. (2.1). If the analogy to the scalar case holds, this simple Fock-type parabolic approximation should yield significant information about the propagation of elastic waves in media with relatively small and slowly varying inhomogeneity.

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Group representations in the Liouville representation and the algebraic approach

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Group representations on the Liouville representation spaces are considered. It is shown that the state space $\mathscr{T}_1(H)$ of trace class operators on Hilbert space H and the observable space $\mathscr{L}(H)$ of bounded operators are completely reducible under physically induced representations of compact Hausdorff groups when appropriate topologies are used. For state space $\mathscr{T}_1(H)$ both the norm topology and the weak topology lead to complete reducibility, while for observable space $\mathscr{L}(H)$ the weak-$*$ topology—but not the norm topology—suffices. This leads to conservation laws, selection rules, and Wigner–Eckart theorems for the Liouville representation. It is shown that serious difficulties are encountered when a similar theory is attempted on the observable space and state space used in the algebraic approach.

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I. INTRODUCTION

Symmetry principles play a fundamental role in the understanding of physical laws and physical systems. Symmetry operations are conveniently represented in terms of group operations on objects representing the states and/or the observables of a system. When the states of a quantum mechanical system are represented by vectors in a Hilbert space H, most symmetry operations are represented by unitary operators, and a wealth of information may be obtained by applying the well-developed theory of unitary group representations. In this way one may derive conservation laws, selection rules, and quantitative relationships among certain transition amplitudes.

More recently, alternative phenomenologically oriented formulations of quantum mechanics have proven useful. They have the advantages of being formulated in terms of operationally defined quantities and of treating pure and mixed states on the same basis. One of these, the Liouville representation, is a straightforward generalization of the standard Hilbert space formulation in that it represents pure or mixed states as density operators on a fundamental Hilbert space H. Another, the algebraic approach, is defined more abstractly and has the property that it includes many more states than the Liouville representation. Both of these formulations are vector space theories, in which the vector spaces representing the states and observables are Banach spaces. Accordingly, while symmetry operations can be represented by operators acting on the space of states or the space of observables, they cannot be represented by unitary operators acting on these spaces; the theory of unitary group representations cannot be directly applied. Nevertheless, it is reasonable to expect that symmetry arguments will provide physical information similar to that which they provide in the pure state (i.e., Hilbert space) representation. Indeed, since the Banach space representations contain all information present in the Hilbert space representation, one might reasonably expect to obtain even stronger results. We show here that in fact there are conservation laws and selection rules for transitions which may be derived directly from group representations on the Liouville representation spaces which may only be obtained indirectly in the pure state-Hilbert space representation, where one applies group methods to the wavefunctions and then constructs averages over suitable mixed states.

In this paper we begin an investigation of representations of symmetry groups on the Banach spaces occurring in the Liouville representation and in the algebraic approach. We will restrict our attention to compact symmetry groups and deal primarily with the Liouville representation. We begin in Sec. II by recalling the fundamental results from the theory of unitary representations of compact groups on Hilbert spaces which are necessary to establish the desired physical results (e.g., conservation laws, selection rules, and Wigner–Eckart type theorems). We then show that the necessary mathematical results do not extend to the general continuous representation of a compact group on a Banach space. Thus, in order to draw the desired physical conclusions, it is necessary to establish these important results for the specific representations which are encountered in physical applications. In preparation for this, Sec. III reviews the Liouville space formulation of quantum theory, while Sec. IV is devoted to general aspects of group representations on topological vector spaces. In Sec. V we show that appropriate topologies make the state space and observable space of the Liouville representation completely reducible. This leads

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to conservation laws, selection rules, and Wigner–Eckart type theorems for statistical properties describing quantum mechanical ensembles. These results may be obtained only indirectly (through explicit averaging procedures) from the application of group theory at the wavefunction (i.e., pure state) level. Finally in Sec. VI we show that difficulties are encountered when one attempts to generalize the unitary representation results to the representations occurring in the algebraic approach.

II. PROPERTIES OF UNITARY REPRESENTATIONS

Central to the theory and application of unitary group representations are the following classical results[1–3] (here G is a separable compact topological group, and all vector spaces are assumed to be complex):

(1) Let $U{:}G \times H \to H$ be a continuous unitary representation of G on Hilbert space H, and let H_1 be a subspace of H which is invariant under U [i.e., $U(g)H_1 \subset H_1$ for all g in G]. Then there exists a closed subspace H_2 of H which is invariant under U and such that H is the direct sum $H = H_1 \oplus H_2$ of H_1 and H_2. In fact, H_2 may be chosen to be the orthogonal complement of H_1 (i.e., $H_2 = H_1^{\perp} = \{v \in H \mid \langle v|v_1\rangle = 0 \text{ for all } v_1 \text{ in } H\}$).

(2) If $U{:}G \times H \to H$ is a continuous unitary representation of G on Hilbert space H which is irreducible (i.e., H has no nontrivial closed invariant subspaces), then H is finite-dimensional.

(3) (Schur's lemma): Let U_1: $G \times H_1 \to H_1$ and U_2: $G \times H_2 \to H_2$ be continuous unitary representations of G on Hilbert spaces H_1 and H_2, respectively. Let $\mathscr{S}: H_1 \to H_2$ be a linear operator from H_1 to H_2 which commutes with the actions of the group [i.e., $\mathscr{S} U_1(g) = U_2(g)\mathscr{S}$ for all g in G; $\mathscr{S}$ is called an *intertwining operator* for U_1 and U_2]. Then, if U_1 and U_2 are irreducible, either $\mathscr{S}$ is the zero operator (i.e., $\mathscr{S}v_1 = 0$ for all v_1 in H_1) or $\mathscr{S}$ is an isomorphism (i.e., one-to-one and onto). In the latter case $\mathscr{S}$ is invertible and we have $U_1(g) = \mathscr{S}^{-1} U_2(g)\mathscr{S}$ and $U_2(g) = \mathscr{S} U_1(g)\mathscr{S}^{-1}$ so that the irreducible representations U_1 and U_2 are equivalent.

(4) (Peter–Weyl)[1–3]: Let $H = L^2(G)$ be the Hilbert space of square integrable functions (relative to Haar measure) on G, and let $U{:}\, G \times H \to H$ be the right regular representation of G defined by $[U(g)f](h) = f(hg)$, where g and h are in G. Then H may be decomposed into a direct sum of irreducible representations in which each unitary irreducible representation of G occurs with a (finite) multiplicity equal to its dimension. Thus, recalling that the dual object $\hat{G}$ of G is the collection of (equivalence classes of) irreducible unitary representations of G, we have

$$L^2(G) = \sum_{\hat{g} \in \hat{G}} \oplus \sum_{i=1}^{\dim(\hat{g})} \oplus H_{\hat{g}},$$

where $H_{\hat{g}}$ is a representation space for representation $\hat{g}$ and $\dim(\hat{g})$ is its dimension.

(5) (A. Gurevic[4]): If $U{:}G \times H \to H$ is a continuous unitary representation of G on Hilbert space H, then U is completely reducible. That is, for each $\hat{g} \in \hat{G}$ there is a cardinal number $m_{\hat{g}}$ such that $H = \Sigma_{\hat{g} \in \hat{G}} \oplus m_{\hat{g}} H_{\hat{g}}$, where $m_{\hat{g}} H_{\hat{g}}$ is the direct sum of $m_{\hat{g}}$ copies of $H_{\hat{g}}$. Each $m_{\hat{g}} H_{\hat{g}}$ is a primary subrepresentation of H, and, if $\hat{g} \neq \hat{g}'$, then $m_{\hat{g}} H_{\hat{g}}$ and $m_{\hat{g}'} H_{\hat{g}'}$ are disjoint. (Recall that two representations are *disjoint* if there exists no nonzero intertwining operator between them, and that a representation is *primary* if it cannot be decomposed into a direct sum of disjoint representations.)

(6) (Racah[5,6]): If G is a Lie group, there is a finite set of operators (the generalized Casimir invariants) whose eigenvalues uniquely characterize (to within equivalence) the irreducible representations of G. Thus the primary subrepresentations $m_{\hat{g}} H_{\hat{g}}$ of a unitary representation may be labeled by the eigenvalues of the generalized Casimir operators on the irreducible representation $\hat{g}$. Moreover the representations of the Casimir invariants are self-adjoint.

Conservation laws, selection rules, and Wigner–Eckart theorems may be easily derived from these results. By the theorem of Gurevic the Hilbert space of state vectors is reducible into a direct sum of primaries corresponding to each irreducible representation of G. Now a symmetry operation is by definition an invertible operation on a physical system which commutes with time development. That is, if one starts at time t_0 with two identical systems (A and B) and performs a symmetry operation on system A at time $t_A > t_0$ and the same symmetry operation on system B at time $t_B > t_0$, then at any time t greater than both t_A and t_B the two systems are again identical. Thus, if one has a group of symmetry operations the time translation operator $U(t_2, t_1)$ from t_1 to t_2 for any pair of times t_1 and t_2 commutes with the group of symmetry operations, i.e., $U(t_2, t_1)$ is an intertwining operator. Consequently, the transition amplitude $\langle \phi_{\hat{g}'} | U(t_2, t_1) | \psi_{\hat{g}} \rangle$ from any state $\psi_{\hat{g}}$ in primary $m_{\hat{g}} H_{\hat{g}}$ to any state $\phi_{\hat{g}'}$ in a different (i.e., disjoint) primary $m_{\hat{g}'} H_{\hat{g}'}$ is zero (by definition of disjoint representations). Because the Casimir operators are self-adjoint, they represent observables; we see that the values of these observables are conserved.

Selection rules and Wigner–Eckart theorems may be derived similarly. Suppose that one has a system made up of two subsystems (A and B). The Hilbert space H of pure states of the system is the tensor product $H = H_A \otimes H_B$ of the Hilbert spaces describing the subsystems. Each of these spaces has a direct sum decomposition into disjoint primaries; $H = \Sigma_{\hat{g} \in \hat{G}} m_{\hat{g}} H_{\hat{g}}$, $H_A = \Sigma_{\hat{g} \in \hat{G}} m^A_{\hat{g}} H_{\hat{g}}$, and $H_B = \Sigma_{\hat{g} \in \hat{G}} m^B_{\hat{g}} H_{\hat{g}}$. Suppose that at time t_0 subsystem A is described by vector $\phi^A_{\hat{g}_A}$ in primary $\hat{g}_A$ and subsystem B is described by vector $\phi^B_{\hat{g}_B}$ in primary $\hat{g}_B$. Then the transition amplitude $\langle \psi_{\hat{g}} | U(t_2, t_1) | \phi^A_{\hat{g}_A} \otimes \phi^B_{\hat{g}_B} \rangle$ into a state $\psi_{\hat{g}}$ of the entire system in primary $\hat{g}$ will be zero unless the irreducible representation $\hat{g}$ is contained in the product $\hat{g}_A \times \hat{g}_B$. This provides selection rules for changes in the eigenvalues of the generalized Casimir invariants. Furthermore, the Wigner–Eckart theorem is obtained from Schur's lemma which implies that any intertwining operator [such as the time translation operator $U(t_2, t_1)$] depends upon only one parameter for each irredicuble subspace in H and each pair of irreducible subspaces in H_A and H_B.

It is clear that if the six results listed above can be extended to representations on Banach spaces, then conservation laws, selection rules, and Wigner–Eckart theorems are valid for the Banach space representations of quantum theory. Accordingly, we will see which of these results generalize to isometric representations on Banach spaces. First of all, it is not ture that every closed invariant subspace B_1 of a continuous isometric representation $\mathscr{U}: G \times B \to B$ may be complemented by a closed invariant subspace B_2 such that $B = B_1 \oplus B_2$. In particular, let $B = \mathscr{L}(H)$ be the Banach space of bounded operators on Hilbert space H; let $B_1 = \mathrm{Com}(H)$ be the Banach space of compact operators on H. Then, if $U: G \times H \to H$ is a continuous unitary representation of compact group G on H, $\mathscr{U}: G \times B \to B$ defined by $\mathscr{U}(g)\mathscr{O} = U(g)\mathscr{O}U^{-1}(g)$ is a continuous isometric representation of G on B which leaves B_1 invariant. But B_1 has no complementing subspace[7] in B so it certainly has no invariant complementing subspace. Since establishing the existence of complementary invariant subspaces is a key step in proving the complete reducibility of an arbitrary unitary representation, this failure suggests that not every continuous isometric representation on a Banach space will be completely reducible.

Secondly, while not every continuous irreducible representation of a compact group G on an arbitrary topological vector space is finite-dimensional, this statement is true if the topological vector space has a nonzero continuous linear functional.[3] The Hahn–Banach theorem thus implies that every continuous irreducible representation of G on a Banach space is finite-dimensional.

Thirdly, since by (2) every irreducible representation of G on a Banach space is finite-dimensional, Schur's lemma as stated applies to Banach space representations.

The Peter–Weyl theorem is specifically a Hilbert space result and need not be generalized.

It is not true that every continuous isometric representation $\mathscr{U}: G \times B \to B$ of a compact group is completely reducible. Specifically, the representation of the circle group $S^1 = \{e^{i\theta} | 0 \leqslant \theta < 2\pi\}$ on the space $B = L^1(S^1)$ of integrable functions on S^1 given by $[\mathscr{U}(\theta)f](\phi) = f(\theta + \phi)$ is not completely reducible.[8]

Finally, since the irreducible representations are all finite-dimensional, Racah's theorem on generalized Casimir invariants is unchanged.

Thus, in order to prove the conservation laws, selection rules, and Wigner–Eckart theorems it must be demonstrated that the particular representations encountered in physical applications are in fact completely reducible. We show in Sec. V that the group representations on the spaces of the Liouville representations are completely reducible.

III. THE LIOUVILLE REPRESENTATION

In the Liouville representation each state is represented by an operator ρ on Hilbert space H which satisfies:

DO1. ρ is self-adjoint, i.e., $\rho^\dagger = \rho$.
DO2. ρ is nonnegative, i.e., $\langle\psi|\rho|\psi\rangle \geqslant 0 \ \forall \ \psi \in H$.
DO3. ρ has unit trace, i.e., ρ is trace class and $\mathrm{tr}\rho = 1$.

Any such operator is called a density operator (DO). State space is defined to be the complex vector space spanned by the density operators. It is precisely the Banach space of trace class operators on H and is denoted by $\mathscr{I}_1(H)$. State space thus has a norm (the trace class norm) given by

$$\|A\|_1 = \mathrm{tr}[(A^+A)^{1/2}]. \tag{3.1}$$

Notice that each density operator has a state space norm of one.

Observables are represented by the bounded self-adjoint operators on H. Observable space is defined to be the complex vector space spanned by the observable operators. It is precisely the Banach space of all bounded operators on H and is denoted by $\mathscr{L}(H)$. Observable space thus has a norm (the operator norm) given by

$$\|\mathscr{O}\| = \sup_{\substack{\psi \in H \\ \langle\psi|\psi\rangle = 1}} \langle \mathscr{O}\psi | \mathscr{O}\psi\rangle^{1/2}. \tag{3.2}$$

The expectation value of observable $\mathscr{O}$ when the system is described by density operator ρ is given by $\mathrm{tr}(\mathscr{O}\rho)$. This may be extended to a sesquilinear form on $\mathscr{L}(H) \times \mathscr{I}_1(H)$ by

$$(\mathscr{O}, A) \to \langle\langle \mathscr{O}|A\rangle\rangle \equiv \mathrm{tr}(\mathscr{O}^+A). \tag{3.3}$$

$\mathscr{L}(H)$ is the dual of $\mathscr{I}_1(H)$,[9,10] where the duality is expressed by the sesquilinear form $\langle\langle \ | \ \rangle\rangle$. Furthermore, the norm of bounded operator $\mathscr{O}$ considered as a linear functional on $\mathscr{I}_1(H)$ coincides with its norm when it is considered as a bounded operator on H.[9,10] Thus

$$\|\mathscr{O}\| = \sup_{\substack{A \in \mathscr{I}_1(H) \\ \|A\|_1 = 1}} |\langle\langle \mathscr{O}|A\rangle\rangle|. \tag{3.4}$$

The norm of $A \in \mathscr{I}_1(H)$ is similarly given by[9,10]

$$\|A\|_1 = \sup_{\substack{\mathscr{O} \in \mathscr{L}(H) \\ \|\mathscr{O}\| = 1}} |\langle\langle \mathscr{O}|A\rangle\rangle|. \tag{3.5}$$

The norms $\|\cdot\|_1$ and $\|\cdot\|$ naturally define topologies on state space $\mathscr{I}_1$ and observable space $\mathscr{L}$. However, the duality between state space and observable space provides each with an alternative topology. The weak topology[9,11] on $\mathscr{I}_1$ is defined to be the weakest vector space topology such that for each $\mathscr{O} \in \mathscr{L}$ the expectation value function $E_{\mathscr{O}}^+ : \mathscr{I}_1 \to C$ defined by $E_{\mathscr{O}}^+(A) = \langle\langle \mathscr{O}|A\rangle\rangle$ is continuous. It has the property that for any topological vector space X a linear function $f: X \to \mathscr{I}_1$ is continuous if and only if the composite function $E_{\mathscr{O}}^+ \circ f: X \to C$ is continuous for each $\mathscr{O} \in \mathscr{L}$. Similarly the weak-$*$ topology[9,11] on $\mathscr{L}$ is defined to be the weakest vector space topology such that for each $A \in \mathscr{I}_1$ the expectation value function $E_A : \mathscr{L}_1 \to \mathbb{C}$ defined by $E_A(\mathscr{O}) = \mathrm{tr}\mathscr{O}^+A$ is continuous. It has the property that for any topological vector space X a linear function $f: X \to \mathscr{L}$ is continuous if and only if the composite function $E_A \circ f: X \to \mathbb{C}$ is continuous for each $A \in \mathscr{I}_1$.

State space $\mathscr{I}_1$ with either the norm or the weak topology and observable space with either the norm or weak-$*$ topology are locally convex and Hausdorff.[11]

IV. GROUP REPRESENTATIONS ON TOPOLOGICAL VECTOR SPACES

Throughout this section G is a compact Hausdorff topological group with Haar measure dg, V is a locally convex topological vector space, and $\Pi: G \to \mathscr{L}(V)$ is a group representation on V such that $(g, v) \mapsto \Pi(g)v$ from $G \times V$ to V is jointly continuous. We are most interested in the case where V does not have a Hilbert space structure. We begin by considering direct sum decompositions of V and then define complete reducibility of representation Π.

Definition: Suppose J is a finite index set and that for each $j\in J$ there exists a nonzero linear operator P_j on V such that

ADS 1. $P_iP_j = 0$ if $i\neq j$.
ADS 2. $P_iP_i = P_i$.
ADS 3. $\Sigma_{j\in J}P_j = I$ the identity operator on V.

Then we say we have an *algebraic direct sum (ADS) decomposition* of V and that V is *the algebraic direct sum* of $\{V_j\}_{j\in J}$ and we write $V=\Sigma_{j\in J}\oplus V_j$. Here $V_j = P_jV$ is the range of operator P_j and is an *algebraic direct summand* of V.

Definition: Suppose J is an index set and that for each $j\in J$ there exists a nonzero linear operator P_j on V such that

TDS 1. $P_iP_j = 0$ if $i\neq j$.
TDS 2. $P_iP_i = P_i$.
TDS 3. Each P_j is continuous.
TDS 4. $\Sigma_{j\in J}P_j = I$, where $I\in\mathscr{L}(V)$ is the identity operator on V and the sum converges in the strong operator topology on $\mathscr{L}(V)$ (i.e., for each $v\in V$ and each neighborhood N of v there exists a finite set $J'\subset J$ such that for each finite set $J''\subset J$ satisfying $J'\subset J''$ the finite sum $\Sigma_{j\in J''}P_jv$ is in neighborhood N).

Then we say we have a *topological direct sum (TDS) decomposition* of V and that V is a topological direct sum of $\{V_j\}_{j\in J}$ and we write $V=\Sigma_{j\in J}\oplus V_j$. Here $V_i = P_iV$ is the range of operator P_i and is a *topological direct summand* of V.

Definition: If $V=V_1\oplus V_2$ is an *algebraic* (respectively, *topological*) *direct sum* then V_2 is called an *algebraic* (respectively, *topological*) *complement* of V_1, and vice versa. We also say that V_1 is *complemented* by V_2.

These definitions call for some comment:

(1) When V is finite-dimensional, there is no difference between an algebraic direct sum and a topological direct sum. This is because (a) the index set J is necessarily finite so that no topology is needed to define the sum $\Sigma_{j\in J}P_j$ and (b) on a finite-dimensional vector space every linear operator P_j is continuous.

(2) While every subspace V_1 of V is algebraically complemented by some subspace V_2, it need not have a topological complement even if it is closed. However, V_1 will have a topological complement if it is closed and satisfies any one of the following three conditions[3]:

(a) V_1 has finite codimension,

(b) V_1 has finite dimension (the assumption that V is locally convex is crucial here),

(c) V is linearly homeomorphic with a Hilbert space.

(3) The above definition of topological direct sums does not correspond precisely with the universally defined direct sum. It is, however, simply related to the universal topological direct sum and the universal topological direct product.[12,13]

Definition: Suppose J is an index set and V_j is a topological vector space for each $j\in J$. The *universal topological direct sum* of $\{V_j\}_{j\in J}$ is the (unique) locally convex topological vector space (denoted by $\widetilde{\Sigma}_{j\in J}\oplus V_j$) equipped with a set of continuous linear maps I'_j: $V_j\to\widetilde{\Sigma}_{j\in J}\oplus V_j$ such that the following universal mapping property is satisfied. Given any locally convex topological vector space W and any set of continuous linear maps F_j: $V_j\to W$, there exists a unique continuous linear map F: $\widetilde{\Sigma}_{j\in J}\oplus V_j\to W$ such that $F_j = F\circ I'_j$.

Concretely, $\widetilde{\Sigma}_{j\in J}\oplus V_j$ is the vector space of all functions on J such that $f(j)\in V_j$ and $f(j)=0$ for all but a finite number of $j\in J$. The collection of subsets $\mathscr{O}=\{f\in\widetilde{\Sigma}_{j\in J}\oplus V_j\,|\,f(j)\in\mathscr{O}_j,\ \mathscr{O}_j$ open in $V_j\}$ is a local base at 0 for the universal direct sum topology.

The insertion operators I_j: $V_j\to V=\Sigma_{j\in J}\oplus V_j$, which are restrictions of the identity operator I: $V\to V$ to the closed subspaces V_j are continuous and linear so that by the universal mapping property there exists a continuous linear function I:$\widetilde{\Sigma}_{j\in J}\oplus V_j\to V$ such that $I_j = I\circ I'_j$. I is one-one so $\widetilde{\Sigma}_{j\in J}\oplus V_j$ is isomorphic to a subspace of V. Furthermore the topology on V is weaker than the $\{I_j\}_{j\in J}$-final linear topology on V.

Definition: Suppose J is an index set and V_j is a topological vector space for each $j\in J$. The *universal topological direct product* of the V_j is the (unique) locally convex topological vector space $\widetilde{\Pi}_{j\in J}V_j$ equipped with a set of continuous linear maps π_j:$\widetilde{\Pi}_{j\in J}V_j\to V_j$ such that the following universal mapping property is satisfied. Given any locally convex topological vector space W and any set of continuous linear maps F_j :$W\to V_j$, there exists a unique continuous linear map F:$W\to\widetilde{\Pi}_{j\in J}V_j$ such that $F_j = \pi_j\circ F$.

Concretely $\widetilde{\Pi}_{j\in J}V_j$ is the vector space of all functions on J such that $f(j)\in V_j$. The collection of subsets of the form $\mathscr{O}=\pi_j^{-1}(\mathscr{O}_j)$ for $\mathscr{O}_j$ open in V_j is a subbase for the product topology.

The projection operators P_j: $V=\Sigma_{j\in J}\oplus V_j\to V_j$ are continuous and linear so by the universal mapping property there exists a continuous linear map P: $V\to\widetilde{\Pi}_{j\in J}V_j$ such that $P_j=\pi_j\circ P$. Because no $v\in V$ is annihilated by all P_j, P is one-one and V is isomorphic to a subspace of $\widetilde{\Pi}_{j\in J}V_j$. The topology on V must be stronger than the subspace topology inherited from $\widetilde{\Pi}_{j\in J}V_j$.

The relationship between our definition of a topological direct sum and the universal topological direct sum and universal topological direct product may be summarized as follows: For our purposes a topological direct sum of locally convex spaces $\{V_j\}_{j\in J}$ is any locally convex topological vector space V which is (linearly isomorphic to) a subspace of the universal direct product $\widetilde{\Pi}_{j\in J}V_j$ and which contains the universal direct sum $\widetilde{\Sigma}_{j\in J}\oplus V_j$ as a vector subspace such that the topology on V is stronger than the subspace topology inherited from $\widetilde{\Pi}_{j\in J}V_j$ and such that it induces a topology on the universal direct sum $\widetilde{\Sigma}_{j\in J}\oplus V_j$ which is weaker than the universal direct sum topology.

(4) When the index set J is finite, the universal direct sum and the universal direct product of $\{V_j\}_{j\in J}$ are equal so that any two direct sums of $\{V_j\}_{j\in J}$ are isomorphic.[13] Hence the topological direct sum agrees with the universal topological direct sum.

(5) When the index set J is infinite, the universal direct product is much bigger than the universal direct sum. Consequently, two different vector spaces V and W may be direct sums of the same $\{V_j\}_{j\in J}$. V and W may differ both in terms

of their topologies and in terms of their sets. This nonuniqueness is easily illustrated by taking direct sums of an infinite number of Banach spaces B_j. For all positive p, let B^p be the set of functions f such that $f(j) \in B_j$ and $\|f\|_p = (\Sigma_{j\in J} \|f(j)\|^p)^{1/p}$ is finite. Here $\|f(j)\|$ is the norm of $f(j)\in B_j$. This gives a topological direct sum for each $p>0$. While $p=1$ is sometimes taken as the definition of the Banach space direct sum,[1] there is nothing canonical about this choice.

We conclude this section with three definitions.

Definition: A closed subspace V_1 of V is *invariant* under the representation $\Pi: G \to \mathscr{L}(V)$ if $\pi(g)v_1 \in V_1$ for all $v_1 \in V_1$ and all $g \in G$.

Definition: The representation $\Pi: G \to \mathscr{L}(V)$ is *irreducible* if V has no nontrivial closed invariant subspaces.

Definition: The representation $\Pi: G \to \mathscr{L}(V)$ is *completely reducible* if V has a direct sum decomposition into invariant irreducible subspaces.

V. THE COMPLETE REDUCIBILITY OF $\mathscr{T}_1(H)$ AND $\mathscr{L}(H)$

In this section we prove the main results of this paper: The projection operators from state space (observable space) to the standard irreducible tensorial operators decompose state space (observable space) into a direct sum of invariant subspaces when an appropriate topology is used. We begin by considering the properties of the physically induced representations on state space $\mathscr{T}_1(H)$ and observable space $\mathscr{L}(H)$.

Let $T: G \times H \to H$ be a jointly continuous unitary representation of a compact, Hausdorff group G on Hilbert space H, where H is assumed to have the norm topology. This induces several representation of G on state space $\mathscr{T}_1(H)$. Define, for $A \in \mathscr{T}_1(H)$,

$$\mathscr{T}_1(g)A \equiv T(g)A, \tag{5.1}$$

$$\mathscr{T}_r(g)A \equiv AT^+(g), \tag{5.2}$$

$$\mathscr{T}_a(g)A \equiv T(g)AT^+(g). \tag{5.3}$$

These are the left, right, and adjoint representations of G, respectively. $\mathscr{T}_1$ and $\mathscr{T}_r$ may be combined to form a representation $\mathscr{T}_p$ of the product group $G\times G$ by defining

$$\mathscr{T}_p(g,h)A = T(g)AT^+(h) = \mathscr{T}_1(g)\mathscr{T}_r(h)A. \tag{5.4}$$

The adjoint representation is the product representation restricted to the diagonal: $\mathscr{T}_a(g) = \mathscr{T}_p(g,g)$. Because of the unitarity of T, all of these are isometric representations, i.e.,

$$\|\mathscr{T}A\|_1 = \|A\|_1 \quad \forall A \in \mathscr{T}_1(H). \tag{5.5}$$

For each of the representations $\mathscr{T}_1$, $\mathscr{T}_r$, and $\mathscr{T}_a$ the mapping $(g,A) \mapsto \mathscr{T}(g)A$ is jointly continuous from $G \times \mathscr{T}_1$ to $\mathscr{T}_1$ when $\mathscr{T}_1$ is given either the norm or the weak topology. Similarly the mapping $(g,h,A) \mapsto \mathscr{T}_p(g,h)A$ is jointly continuous from $G\times G\times \mathscr{T}_1$ to $\mathscr{T}_1$. To prove these assertions, assume first that $g \mapsto \mathscr{T}(g)A$ from G to $\mathscr{T}_1$ is norm continuous for each $A \in \mathscr{T}_1$. Then

$$\begin{aligned}
&\|\mathscr{T}(g)A - \mathscr{T}(g_0)A_0\|_1 \\
&\quad \leqslant \|\mathscr{T}(g)(A-A_0)\|_1 + \|[\mathscr{T}(g)-\mathscr{T}(g_0)]A_0\|_1 \\
&\quad = \|A-A_0\|_1 + \|[\mathscr{T}(g)-\mathscr{T}(g_0)]A_0\|_1,
\end{aligned}$$

which goes to zero as $A \to A_0$ and $g \to g_0$ so joint continuity has been established. Thus, since if $g \mapsto \mathscr{T}(g)A$ is norm continuous it is also weakly continuous, it is only necessary to show that it is norm continuous. We first prove this for the left representation. Choose $\epsilon>0$. Let $A = \Sigma_{j\in J} |\phi_i\rangle \lambda_i \langle \psi_i|$ be the polar representation[10] of A. Thus $\langle \phi_i|\phi_j\rangle = \delta_{ij}$, $\langle \psi_i|\psi_j\rangle = \delta_{ij}$, $\lambda_i \geqslant 0$, $\Sigma_{i\in I}\lambda_i = \|A\|_1$ and I is the set of integers. Choose $N \in I$ such that $\Sigma_{i=N+1}^{\infty} \lambda_i < \epsilon/4$ and choose neighborhood $\mathscr{U}$ of g_0 such that $\|[T(g)-T(g_0)]\phi_i\| < \epsilon/2N\lambda_i$ for $i=1,...,N$. Then, defining $A_N = \Sigma_{i=1}^N |\phi_i\rangle\lambda_i\langle\psi_i|$ and $A' = A - A_N$, we have

$$\begin{aligned}
&\|[\mathscr{T}_1(g) - \mathscr{T}_1(g_0)]A\|_1 \\
&\quad \leqslant \|[T(g)-T(g_0)]A_N\|_1 + \|[T(g)-T(g_0)]A'\|_1 \\
&\quad \leqslant \sum_{i=1}^N \lambda_i \|[T(g)-T(g_0)]\phi_i\| + \|T(g)-T(g_0)\|\cdot\|A'\|_1 \\
&\quad < \epsilon/2 + 2(\epsilon/4) = \epsilon.
\end{aligned}$$

A similar argument proves that the right representation $\mathscr{T}_r$ is norm continuous. It is now easy to show that the product representation is continuous, i.e., that $(g,h) \mapsto \mathscr{T}_p(g,h)A$ is continuous for each $A \in \mathscr{T}_1$. Fix $\epsilon>0$. Choose a neighborhood $\mathscr{U}_1$ of g_0 such that $\|[\mathscr{T}_1(g)-\mathscr{T}_1(g_0)]A\|_1 < \epsilon/2$ for all $g\in\mathscr{U}_1$ and a neighborhood $\mathscr{U}_2$ of h_0 such that $\|[\mathscr{T}_r(h) - \mathscr{T}_r(h_0)]A\|_1 < \epsilon/2$ for all $h \in \mathscr{U}_2$. Then

$$\begin{aligned}
&\|[\mathscr{T}_p(g,h) - \mathscr{T}_p(g_0,h_0)]A\|_1 \\
&\quad = \|T(g)AT^+(h) - T(g_0)AT^+(h_0)\|_1 \\
&\quad \leqslant \|T(g)AT^+(h) - T(g)AT^+(h_0)\|_1 \\
&\quad\quad + \|T(g)AT^+(h_0) - T(g_0)AT^+(h_0)\|_1 \\
&\quad = \|A[T^+(h) - T^+(h_0)]\|_1 + \|[T(g)-T(g_0)]A\|_1 \\
&\quad = \|[\mathscr{T}_r(h) - \mathscr{T}_r(h_0)]A\|_1 + \|[\mathscr{T}_1(g) - \mathscr{T}_1(g_0)]A\|_1 < \epsilon.
\end{aligned}$$

The continuity of the adjoint representation $\mathscr{T}_a$ is obtained from the restriction of the product representation $\mathscr{T}_p$ to the diagonal.

Similar representations may be defined on observable space $\mathscr{L}(H)$:

$$\tilde{\mathscr{T}}_1(g)\mathscr{O} = T(g)\mathscr{O}, \tag{5.6}$$

$$\tilde{\mathscr{T}}_r(g)\mathscr{O} = \mathscr{O}T^+(g), \tag{5.7}$$

$$\tilde{\mathscr{T}}_a(g)\mathscr{O} = T(g)\mathscr{O}T^+(g), \tag{5.8}$$

and

$$\tilde{\mathscr{T}}_p(g,h)\mathscr{O} = T(g)\mathscr{O}T^+(h). \tag{5.9}$$

However, these representations are not, in general, norm continuous. Thus, for example, let $H = L^2(R^3)$ be the square integrable functions on Euclidean 3-space, let G be the one-parameter group of rotations about the z axis, and let $[T(\theta)\psi](x,y,z) = \psi(x\cos\theta + y\sin\theta, -x\sin\theta + y\cos\theta, z)$ for $\psi \in L^2(H)$. The infinitesimal generator of T is the angular momentum operator L_z which is not bounded so that $\theta \mapsto T(\theta)$ is not norm continuous, i.e., $\|T(\theta) - I\|$ does not tend to zero as θ tends to zero.[11] This implies that the mapping $\theta \mapsto \tilde{\mathscr{T}}_1(g)I$ is not continuous at $\theta = 0$. Similar examples can be given for the representations $\tilde{\mathscr{T}}_r$, $\tilde{\mathscr{T}}_a$, and $\tilde{\mathscr{T}}_p$. Because they are not norm continuous they are not weakly continuous.[14] They are, however, weak-* continuous; that is, the map

$g \mapsto \tilde{\mathscr{T}}(g)\mathscr{O}$ is continuous when $\mathscr{L}(H)$ is given the weak-$*$ topology. Thus, fix $A \in \mathscr{I}_1(H)$ and $\epsilon > 0$. Because the maps $g \mapsto g^{-1}$ and $g \mapsto \mathscr{T}(g)A$ are continuous there exists a neighborhood $\mathscr{U}$ of g_0 such that $\|[\mathscr{T}(g^{-1}) - \mathscr{T}(g_0^{-1})]A\|_1 < \epsilon/\|\mathscr{O}\|$ for all $g \in \mathscr{U}$. Then

$$
\begin{aligned}
&|\langle\langle \tilde{\mathscr{T}}(g)\mathscr{O}|A\rangle\rangle - \langle\langle \tilde{\mathscr{T}}(h)\mathscr{O}|A\rangle\rangle| \\
&\quad = |\langle\langle \mathscr{O}|[\mathscr{T}(g^{-1}) - \mathscr{T}(g_0^{-1})]A\rangle\rangle| \\
&\quad \leqslant \|\mathscr{O}\|\cdot\|[\mathscr{T}(g^{-1}) - \mathscr{T}(g_0^{-1})]A\|_1 < \epsilon
\end{aligned}
$$

for all $g \in \mathscr{U}$.

We now inquire into the reducibility of these representations. The irreducible subrepresentations of the unitary representation $T: G \to \mathscr{L}(\mathrm{H})$ provide irreducible subrepresentations in $\mathscr{I}_1(H)$ and $\mathscr{L}(H)$. Let $H = \Sigma_{j\in J} \oplus H_j$ be a direct sum decomposition of H into finite-dimensional orthogonal, invariant, irreducible subspaces as guaranteed by the theorem of Gurevic.[4] Let P_j be the continuous self-adjoint projection operator from H to H_j. For each $(j', j'') \in J \times J$ define the operator $\mathscr{P}_{j'j''}$ on $\mathscr{I}_1(H)$ and the operator $\tilde{\mathscr{P}}_{j'j''}$ on $\mathscr{L}(H)$ by

$$\mathscr{P}_{j'j''}A = P_{j'}AP_{j''}, \quad A \in \mathscr{I}_1(H), \tag{5.10}$$

$$\tilde{\mathscr{P}}_{j'j''}\mathscr{O} = P_{j'}\mathscr{O}P_{j''}, \quad \mathscr{O} \in L(H), \tag{5.11}$$

They clearly satisfy the relations

$$\mathscr{P}_{j_1'j_1''}\mathscr{P}_{j_2'j_2''} = P_{j_1'j_1''}\delta_{j_1'j_2'}\delta_{j_1''j_2''}$$

and

$$\tilde{\mathscr{P}}_{j_1'j_1''}\tilde{\mathscr{P}}_{j_2'j_2''} = \tilde{\mathscr{P}}_{j_1'j_1''}\delta_{j_1'j_2'}\delta_{j_1''j_2''}$$

and thus are projection operators. Furthermore, they do not increase the norm

$$\|\mathscr{P}_{j'j''}A\|_1 \leqslant \|A\|_1 \quad \forall A \in \mathscr{I}_1(H), \tag{5.12}$$

$$\|\tilde{\mathscr{P}}_{j'j''}\mathscr{O}\| \leqslant \|\mathscr{O}\| \quad \forall \mathscr{O} \in \mathscr{L}(H), \tag{5.13}$$

and so they are norm continuous. The conditions TDS1, TDS2, and TDS3 are thus satisfied for the families $\mathscr{P}_{j'j''}$ and $\tilde{\mathscr{P}}_{j'j''}$. If TDS4 is also satisfied, then they define topological direct sum decompositions of $\mathscr{I}_1(H)$ and $\mathscr{L}(H)$, respectively.

We show first that TDS4 is satisfied for the operators $\mathscr{P}_{j'j''}$ on $\mathscr{I}_1(H)$ when $\mathscr{I}_1(H)$ is given the norm topology. It then follows trivially that TDS4 is also satisfied if $\mathscr{I}_1(H)$ is given the weak topology. Let A be in $\mathscr{I}_1(H)$, and let $A = \Sigma_{i\in I} |\phi_i\rangle\lambda_i\langle\psi_i|$ be its polar decomposition. For any pair of finite subsets J' and J'' of J, let

$$A^{(J',J'')} = \sum_{(j',j'')\in J'\times J''} \mathscr{P}_{j'j''}A = \sum_{(j',j'')\in J'\times J''} \mathscr{P}_{j'}A\mathscr{P}_{j''}$$

and let $\psi^{J'} = \Sigma_{j'\in J'}\mathscr{P}_{j'}\psi$ for ψ in H. Choose N so that $\Sigma_{i=N+1}^{\infty} 2\lambda_i < \epsilon/2$ and choose a finite subset K of J so that $N\lambda_{\max}(\|\psi_i - \psi_i^{J''}\|_H + \|\phi_i - \phi_i^{J'}\|_H) < \epsilon/2$ for all finite subsets J' and J'' of J containing K and for all $i \leqslant N$, where $\lambda_{\max} = \sup_{i\in I}\lambda_i$. Then for all $B \in \mathscr{L}(H)$ with $\|B\| = 1$ we have

$$
\begin{aligned}
&|\langle\langle B|A\rangle\rangle - \langle\langle B|A^{J'J''}\rangle\rangle| \\
&\quad = \left|\sum_{i\in I}\lambda_i(\langle\psi_i|B|\phi_i\rangle - \langle\psi_i^{J''}|B|\phi_i^{J'}\rangle)\right| \\
&\quad \leqslant \sum_{i\in I}\lambda_i|\langle\psi_i|B|\phi_i\rangle - \langle\psi_i^{J''}|B|\phi_i^{J'}\rangle| \\
&\quad = \sum_{i\in I}\lambda_i|\langle\psi_i - \psi_i^{J''}|B|\phi_i\rangle + \langle\psi_i^{J''}|B|\phi_i - \phi_i^{J'}\rangle| \\
&\quad \leqslant \sum_{i\in I}\lambda_i(\|\psi_i - \psi_i^{J''}\|_H + \|\phi_i - \phi_i^{J'}\|_H) \\
&\quad \leqslant \sum_{i=1}^{N}\lambda_i(\|\psi_i - \psi_i^{J''}\|_H + \|\phi_i - \phi_i^{J'}\|_H) + \sum_{i=N+1}^{\infty} 2\lambda_i \\
&\quad \leqslant \epsilon
\end{aligned}
$$

for all finite subsets J' and J'' of J containing K. This shows, by virtue of (3.5), that

$$\sum_{(j',j'')\in J\times J} \mathscr{P}_{j'j''}A$$

converges to A in $\mathscr{I}_1(H)$ norm for all A in $\mathscr{I}_1(H)$.

On $\mathscr{L}(H)$ the situation is somewhat different. Since the norm closure of the set of finite rank operators is the set of compact operators and since for every $\mathscr{O} \in \mathscr{L}(H)$ and every finite subset $J' \times J'' \subset J \times J$ the operator

$$\tilde{\mathscr{P}}_{j'j''}\mathscr{O} = \sum_{(j',j'')\in J'\times J''} \tilde{\mathscr{P}}_{j'j''}\mathscr{O} = P_{J'}\mathscr{O}P_{J''}$$

has finite rank, TDS4 will not be satisfied if H is infinite-dimensional and $\mathscr{L}(H)$ is given the norm topology. However, TDS4 is satisfied if $\mathscr{L}(H)$ is given the weak-$*$ topology. Thus choose $A \in \mathscr{I}_1(H)$. Then

$$
\begin{aligned}
&|\langle\langle \tilde{\mathscr{P}}_{j'j''}\mathscr{O}|A\rangle\rangle - \langle\langle \mathscr{O}|A\rangle\rangle| \\
&\quad = |\langle\langle \mathscr{O}|(\mathscr{P}_{j'j''} - I)A\rangle\rangle| \\
&\quad \leqslant \|\mathscr{O}\|\cdot\|(\mathscr{P}_{j'j''} - I)A\|_1,
\end{aligned}
$$

which converges to zero since $\|(\mathscr{P}_{j'j''} - I)A\|_1$ converges to zero.

Let $\mathscr{I}_1^{j'j''}$ be the range of $\mathscr{P}_{j'j''}$ and let $\mathscr{L}^{j'j''}$ be the range of $\tilde{\mathscr{P}}_{j'j''}$. To review, $\mathscr{I}_1(H)$ and $\mathscr{L}(H)$ have the direct sum decompositions

$$\mathscr{I}_1 = \sum_{(j',j'')\in J\times J} \oplus \mathscr{I}_1^{j'j''}, \tag{5.14}$$

$$\mathscr{L}(H) = \sum_{(j',j'')\in J\times J} \oplus \mathscr{L}^{j'j''}. \tag{5.15}$$

Each $\mathscr{I}_1^{j'j''}$ is a finite-dimensional subspace of $\mathscr{I}_1$ which is invariant under the representations $\mathscr{T}_1$, $\mathscr{T}_r$, $\mathscr{T}_a$, and $\mathscr{T}_p$. Similarly each $\mathscr{L}^{j'j''}$ is a finite-dimensional subspace of $\mathscr{L}(H)$, which is invariant under the representations $\tilde{\mathscr{T}}_1$, $\tilde{\mathscr{T}}_r$, $\tilde{\mathscr{T}}_a$, and $\tilde{\mathscr{T}}_p$. The subspaces $\mathscr{I}_1^{j'j''}$ and $\mathscr{L}^{j'j''}$ are obviously irreducible under the product representations $\mathscr{T}_p$ and $\tilde{\mathscr{T}}_p$, respectively. Since they are finite-dimensional, they may be decomposed into irreducible subspaces for each of the other representations using familiar finite-dimensional techniques. (The irreducible subspaces thus obtained consist of the standard irreducible tensorial operators.) Consequently, state space $\mathscr{I}_1(H)$ and observable space $\mathscr{L}(H)$ are completely reducible under the left, right, adjoint, and product representations of the compact and Hausdorff group G.

The set of operators in $\mathscr{L}^{j'j''}$ is identical to the set of operators in $\mathscr{I}^{j'j''}$, and $\mathscr{L}^{j'j''}$ and $\mathscr{I}^{j'j''}$ are isomorphic vector spaces. The fact that the nonisomorphic vector spaces $\mathscr{L}(H)$ and $\mathscr{I}_1(H)$ are the direct sums of these isomorphic vector spaces is possible because of the nonuniqueness of infinite direct sums as explained in Sec. IV.

VI. REPRESENTATION THEORY ON THE SPACES OF THE ALGEBRAIC APPROACH

The algebraic approach[15,16] is a quantum mechanical formalism which is closely related in spirit to the Liouville representation approach. It differs from the Liouville representation in that the space of states is defined to be the set of *all* positive linear functionals ϕ on the set of observables such that $\phi(I) = 1$. Although the spaces of the algebraic approach are defined abstractly, a concrete realization of the axiomatic system is provided by representing each observabe by a self adjoint element of $\mathscr{L}(H)$ for some Hilbert space H. The states are then represented by elements in the dual space $\mathscr{L}^*(H)$. This dual space is a topological direct sum[10]

$$\mathscr{L}^*(H) = \mathscr{I}_1(H) \oplus \mathrm{Com}(H)^\perp$$

of the trace class operators $\mathscr{I}_1(H)$ and the space $\mathrm{Com}(H)^\perp$ of linear functionals which vanish on the compact operators. Thus, whenever H is infinite-dimensional, the set of states used in the algebraic approach is much larger than the set of states used in the Liouville representation. In this section we consider the difference this enlarged state space has on the group representations.

The representations $\tilde{\mathscr{T}}_1, \tilde{\mathscr{T}}_r, \tilde{\mathscr{T}}_a$, and $\tilde{\mathscr{T}}_p$ defined in Eqs. (4.6)–(4.9) still exist on $\mathscr{L}(H)$. These may be used to define representations on $\mathscr{L}^*(H)$ by

$$\begin{aligned}
\tilde{\tilde{\mathscr{T}}}_1(g) &= \tilde{\mathscr{T}}_1^\dagger(g^{-1}),\\
\tilde{\tilde{\mathscr{T}}}_r(g) &= \tilde{\mathscr{T}}_r^\dagger(g^{-1}),\\
\tilde{\tilde{\mathscr{T}}}_a(g) &= \tilde{\mathscr{T}}_a^\dagger(g^{-1}),\\
\tilde{\tilde{\mathscr{T}}}_p(g,h) &= \tilde{\mathscr{T}}_p^\dagger(g^{-1},h^{-1}),
\end{aligned}$$

where $\dagger$ refers to the adjoint operation.

In the algebraic approach there are two natural topologies to consider on $\mathscr{L}(H)$ and $\mathscr{L}^*(H)$. On $\mathscr{L}(H)$ it is natural to consider the norm topology and the weak (Banach space) topology. Both of these topologies are finer than the weak-$*$ topology which is natural in the Liouville representation. On $\mathscr{L}^*(H)$ it is natural to consider the norm topology and the weak-$*$ topology. We must now ask if the representations $\tilde{\mathscr{T}}$ and $\tilde{\tilde{\mathscr{T}}}$ are continuous in any of these topologies. We have already seen that the representations $\tilde{\mathscr{T}}$ on $\mathscr{L}(H)$ are not norm-continuous for many physically significant groups such as one-parameter rotation groups. These one-parameter subgroups cannot be weakly continuous either since weak continuity implies norm continuity.[14] This in turn implies that $\tilde{\tilde{\mathscr{T}}}$ on $\mathscr{L}^*(H)$ cannot be weak-$*$ continuous which implies that $\tilde{\tilde{\mathscr{T}}}$ cannot be norm continuous. In our opinion the failure of these representations to be continuous in physically significant topologies represents, for certain applications, a significant disadvantage of the algebraic approach relative to the Liouville representation approach in which the corresponding representations are continuous.

Since the representations $\tilde{\mathscr{T}}$ and $\tilde{\tilde{\mathscr{T}}}$ are not, in general, continuous, it is difficult to proceed with a general representation theory. It is clear, moreover, that even when $\tilde{\mathscr{T}}$ is continuous the general observable $\mathscr{O} \in \mathscr{L}(H)$ cannot be expanded in terms of irreducible tensorial operators in either a norm convergent or a weak convergent sense. This is because each irreducible tensorial operator is of finite rank. The limit of such operators in either the norm or the weak topology is a compact operator. Thus, unless observable $\mathscr{O}$ is compact, it cannot be expanded in terms of irreducible tensorial operators.

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Inverse scattering. IV. Three dimensions: generalized Marchenko construction with bound states, and generalized Gel'fand–Levitan equations

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This paper represents the final installment in a series on the solution of the inverse scattering problem for the Schrödinger equation in three dimensions. The potential is constructed from a given scattering amplitude without assuming its existence, even in the presence of bound states. For exponentially decreasing potentials, properties of the Jost function and of the regular solution are derived that are sufficient to establish the triangularity of the kernel on which the generalized Gel'fand–Levitan (GL) equation is based. Other generalized GL equations, for nonzero reference potentials, and a nonlinear equation are derived, and for central potentials they are shown to reduce to the well-known radial equations. The contents of the series of papers is summarized.

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1. INTRODUCTION

This paper is the third in a series of papers,[1,2] (referred to in this paper as II and III) on the inverse scattering problem for the Schrödinger equation in three dimensions, with a potential for which no assumption of spherical symmetry is made. In Sec. 2 we discuss four Hilbert problems for operator-valued functions with operator-valued solutions. The results there found are needed for the construction of a potential if there are bound states and for the construction of the Jost function.

Section 3 completes the construction of a potential from a given scattering amplitude that is not known to be associated with an underlying potential, in the presence of bound states. Theorem 3.1 therefore generalizes Theorem 3.1 of III to the case with bound states. It shows that the *miracle*, as defined in II, is a necessary and sufficient condition for the existence of an underlying local potential even when there are bound states. Together with the other assumptions listed for the Class $\mathscr{A}$ in Sec. 3 of III it therefore serves as a characterization of admissible scattering amplitudes. (However, the theorem does not determine the asymptotic fall-off of the potential.)

In Sec. 4 the Jost function is constructed from the given S matrix by solving a Hilbert problem as in Sec. 2. The result is stated in Theorem 4.1. In preparation for the generalized Gel'fand–Levitan equation the Jost function is then expanded on the basis of the spherical harmonics, after a similar expansion of the scattering amplitude. It is shown that if the potential decreases asymptotically exponentially then the spherical-harmonic coefficients of the scattering amplitude behave near $k = 0$ as in (4.13). As a result the coefficients of the Jost function in general behave as in (4.25), though we have not been able to rule out the "accidental" possibility of exceptions if the rank of the coefficients of an infinite set of linear equations is finite and small enough.

The regular solution defined in II is examined in Sec. 5. On the basis of the results of Sec. 4 we find that its spherical-harmonic coefficients behave near $k = 0$ as in (5.2), a fact that for central potentials is well known and easily provable for a large class of potentials irrespective of their asymptotic fall-off. Here, however, a definition of the regular solution by means of a boundary condition is lacking and (5.2) has to be established via the scattering amplitude. The result is Theorem 5.1.

The properties of the regular solution found in Sec. 5 allow us in Sec. 6 to establish the triangularity of its three-dimensional Fourier transform that had been assumed without proper foundation[3] in Sec. 8 of II as a basis for the generalized GL equation. Two versions of this equation are derived. Their kernels are expected, in general, to be distributions.

In Sec. 7 we formally derive generalized GL equations for comparison potentials other than zero, and a generalized nonlinear GL equation. Section 8 contains the reduction of the generalized GL equation to the well known radial equations for central potentials. Section 9 gives a summary of what has been accomplished in the series of papers II, III, and the present one.

2. THE HILBERT PROBLEMS

In this section we shall prepare both the construction of the Jost function and of an underlying potential, if it exists, from a given scattering amplitude in the presence of bound states, by means of the generalized Marchenko equation. It turns out to be necessary for the latter purpose to formulate the Hilbert problem for operator-valued solutions, just as for the Jost function, instead of for vector-valued solutions as in Sec. 4 of II. We therefore pose first four different relevant Hilbert problems. Let $\mathscr{B}$ the class of linear operators on $L^2(S^2)$.

Hilbert Problem $H_0^1(S)$: Suppose a function $S(k)$, $\mathbb{R}\rightarrow\mathscr{B}$, is given and for almost all k it has the following properties[4]: $SS^+ = S^+S = \mathbb{1}$; $S(-k) = S^*(k)$; $QSQ = \widetilde{S}$; $(S - \mathbb{1})\in SL^2(\mathbb{R})$. Find a function $F(k)$, $\mathbb{R}\rightarrow\mathscr{B}$, with the fol-

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lowing properties:

(a) $F(-k) = S^{\dagger}(k) Q F(k) Q;$ (2.1)

(b) $(F - \mathbb{1}) \in SL^2(\mathbb{R});$

(c) $F(k)$ is the boundary-value of an analytic function[5] $F(k)$, $\mathbb{C}^+ \to \mathscr{B}$, holomorphic in $\mathbb{C}^+$;

(d) for $\operatorname{Im} k > 0$, $\lim_{|k| \to \infty} \|F(k) - \mathbb{1}\| = 0.$

Hilbert Problem $H_0^0(S)$: This is identical with $H_0^1(S)$, except that (d) is replaced by: for $\operatorname{Im} k > 0$, $\lim_{|k| \to 0} \|F(k)\| = 0$, and (b) is replaced by: $F \in SL^2(\mathbb{R})$.

Hilbert Problem $H_n^1(S)$: Suppose $S(k)$ is given as in $H_0^1(S)$; also given is a set of n pairs, each consisting of a positive number κ_m and a finite-dimensional subspace $\mathscr{H}_m$ of $L^2(S^2)$, $m = 1,...,n$. Find a function $F(k)$, $\mathbb{R} \to \mathscr{B}$, with the properties (a), (b), and (d) of $H_0^1(S)$, as well as

(c) $F(k)$ is the boundary value of an analytic function $F(k)$, $\mathbb{C}^+ \to \mathscr{B}$, meromorphic in $\mathbb{C}^+$ with simple poles at $k = i\kappa_m$ and residues $I^{(m)}$ there such that[6] $\operatorname{Ran} I^{(m)} = \mathscr{H}_m$.

Hilbert Problem $H_n^0(S)$: This is identical with $H_n^1(S)$, except that (b) and (d) are replaced as in $H_0^0(S)$.

Problem $H_0^1(S)$ is solved by the generalized Marchenko equation. We state the result in the form of

Lemma 2.1: Suppose that $A(k;\theta,\theta')$ is such that the self-adjoint operator $\mathscr{G}$ on $L^2(\mathbb{R}_+ \times S^2)$ whose kernel is given by

$$\begin{aligned} G(\alpha,\beta;\theta,\theta') &= G(\alpha+\beta;\theta,\theta') \\ &= \frac{-i}{(2\pi)^2} \int_{-\infty}^{\infty} dk\, k A^*(k; -\theta',\theta) e^{ik(\alpha+\beta)} \end{aligned} \quad (2.2)$$

is compact, and so is the operator $\mathscr{G}'$ whose kernel is $G'(\alpha,\beta;\theta,\theta') = -G(-\alpha-\beta;\theta,\theta')$; suppose further that the function $G(\alpha)$, $\mathbb{R} \to \mathscr{B}$, defined by the kernel $G(\alpha,\theta,\theta')$, is in $SL^2(\mathbb{R})$ and that neither $\mathscr{G}$ nor $\mathscr{G}'$ has the eigenvalues ± 1. Then $H_0^1(\mathbb{1} - (k/2\pi i)A)$ has a unique solution $F(k)$ given by

$$F(k) = \mathbb{1} + \int_0^{\infty} d\alpha\, e^{ik\alpha} E(\alpha),$$

where for $\alpha \geqslant 0$, $E(\alpha)$ is the unique solution in $SL^2(\mathbb{R}_+)$ of the integral equation

$$E(\alpha) = G(\alpha) Q + \int_0^{\infty} d\beta\, G(\alpha+\beta) E(\beta) Q. \quad (2.3)$$

Furthermore, (2.3) is solvable by iteration, $[F(k)]^{-1}$ has no singularities in $\mathbb{C}^+$, and $(\widetilde{F}^{-1} - \mathbb{1}) \in SL^2(\mathbb{R})$.

Proof: The proof of the first part is entirely analogous to the corresponding part of Theorem 3.1 of III and need not be repeated. The proof of the convergence of the iteration (Neumann series) is contained in that of Theorem 2.1 of III. We need only prove the last part.

Consider the equation for $\alpha > 0$,

$$\widehat{E}(\alpha) = G(-\alpha) Q + \int_0^{\infty} d\beta\, G(-\alpha-\beta) \widehat{E}(\beta) Q. \quad (2.3')$$

By the definition of $\mathscr{G}'$ and the first part of Lemma 2.1 this equation has a unique solution $\widehat{E}(\alpha)$ in $SL^2(\mathbb{R}_+)$ if $\mathscr{G}'$ does not have the eigenvalue -1, and if $\mathscr{G} = (\mathscr{G}')'$ does not have the eigenvalue -1 either then the function $\widehat{F}(k)$ obtained from $\widehat{E}(\alpha)$ by

$$\widehat{F}(k) = \mathbb{1} + \int_0^{\infty} d\alpha\, e^{ik\alpha} \widehat{E}(\alpha)$$

solves the Hilbert problem $H_0^1(S^*)$. Therefore $(\widehat{F} - \mathbb{1}) \in SL^2(\mathbb{R})$ and $\widehat{F}(k)$ is holomorphic in $\mathbb{C}^+$. Furthermore it satisfies the equation

$$\widehat{F}(-k) = \widetilde{S}(k) Q \widehat{F}(k) Q, \quad (2.4)$$

whereas $F(k)$ satisfies (2.1), the transpose of which reads

$$\widetilde{F}(-k) = Q \widetilde{F}(k) Q (S^*)(k). \quad (2.1')$$

Multiplying (2.4) by (2.1') and using the unitarity of S yields

$$\widetilde{F}(-k) \widehat{F}(-k) = Q \widetilde{F}(k) \widehat{F}(k) Q.$$

The left-hand side being holomorphic in $\mathbb{C}^-$ and the right-hand side in $\mathbb{C}^+$ allows us to conclude by an operator generalization of Liouville's theorem that $\widetilde{F}\widehat{F} = \mathbb{1}$, since both $\widehat{F}$ and $\widetilde{F}$ tend to $\mathbb{1}$ as $|k| \to \infty$ in $\mathbb{C}^+$. This concludes the proof.

Corollary: Under the hypotheses of Lemma 2.1 the only solution of $H_0^0(S)$ is the trivial one, $F = 0$.

We now want to solve $H_n^1(S)$. For that purpose we construct the operator $\Pi(k)$ as defined in Sec. 4 of III, by means of κ_m and $\mathscr{H}_m$, $m = 1,...,n$. Then define

$$S^{\text{red}}(k) = Q\, [\Pi(k)]^{-1} Q S(k) \Pi(-k) \quad (2.5)$$

and pose $H_0^1(S^{\text{red}})$ (where red stands for reduced). If S has the properties stated in $H_0^1(S)$ then so does S^{red}. Next construct G^{red} from S^{red} as stated in Lemma 2.1. If $\mathscr{G}^{\text{red}}$ and $\mathscr{G}^{\text{red}\prime}$ are compact, neither has the eigenvalue 1, and $G^{\text{red}}(\alpha) \in SL^2(\mathbb{R})$, then the equation

$$E^{\text{red}}(\alpha) = G^{\text{red}}(\alpha) Q + \int_0^{\infty} d\beta\, G^{\text{red}}(\alpha+\beta) E^{\text{red}}(\beta) Q \quad (2.3'')$$

has a unique solution in $SL^2(\mathbb{R}_+)$ and by Lemma 2.1 the function

$$F^{\text{red}}(k) = \mathbb{1} + \int_0^{\infty} d\alpha E^{\text{red}}(\alpha) e^{ik\alpha} \quad (2.6)$$

is the unique solution of $H_0^1(S^{\text{red}})$. The function

$$F(k) = \Pi(k) F^{\text{red}}(k) \quad (2.7)$$

then solves $H_n^1(S)$.

The function $F(k)$ is, in fact, the only solution of $H_n^1(S)$. Suppose there were two solutions. Then their difference Δ would solve $H_n^0(S)$ and Π^{-1} would solve $H_0^0(S^{\text{red}})$. Hence by the corollary to Lemma 2.1, $\Delta = 0$. Thus we have proved

Lemma 2.2: if $\mathscr{G}^{\text{red}}$ and $\mathscr{G}^{\text{red}\prime}$ are compact, neither has the eigenvalue 1, and $G^{\text{red}} \in SL^2(\mathbb{R})$, then $H_n^1(S)$ has the unique solution $F = \Pi F^{\text{red}}$, where F^{red} is given by (2.6) in terms of the unique solution in $SL^2(\mathbb{R}_+)$ of (2.3'').

Corollary: Under the hypotheses of Lemma 2.2 $H_n^0(S)$ has only the trivial solution $F = 0$.

We now take the Fourier transform of (2.1) in $H_n^1(S)$. Defining

$$E(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{-ik\alpha} [F(k) - \mathbb{1}] \quad (2.8)$$

we obtain

$$E(\alpha) = QE(-\alpha)Q + G(\alpha)Q + \int_{-\infty}^{\infty} d\beta\, G(\alpha+\beta)E(\beta)Q \tag{2.9a}$$

together with the requirement that for $\alpha < 0$

$$E(\alpha) = i\sum_{m=1}^{n} I^{(m)} e^{\alpha\kappa_m}. \tag{2.9b}$$

The system (2.9), in which $G(\alpha)$ and $\kappa_m, \mathscr{H}_m = \operatorname{Ran} I^{(m)}$, $m = 1,...,n$, are given, is equivalent to the demands made in $H_n^1(S)$ on

$$F(k) = \mathbb{1} + \int_{-\infty}^{\infty} d\alpha\, E(\alpha)e^{ik\alpha}. \tag{2.6'}$$

That is, if and only if $E \in SL^2(\mathbb{R})$ and it solves the system (2.9), $F(k)$ of (2.6') solves $H_n^1(S)$.

Suppose that the *homogeneous* system consisting of (2.9b) (in which κ_m and $\mathscr{H}_m = \operatorname{Ran} I^{(m)}$, $m = 1,...,n$, are given) and the equation

$$E(\alpha) = QE(-\alpha)Q + \int_{-\infty}^{\infty} d\beta\, G(\alpha+\beta)E(\beta)Q \tag{2.9'a}$$

had a nontrivial solution. Then the system (2.9) would not have a unique solution. Hence if S satisfies the hypotheses of Lemma 2.2 that lemma would be violated. We have therefore proved

Lemma 2.3: If S is such that $G^{\text{red}} \in SL^2(\mathbb{R})$ and $\mathscr{G}^{\text{red}}$ and $\mathscr{G}^{\text{red}\prime}$ are compact operators without the eigenvalue 1, then the only solution of the homogeneous system (2.9'a) and (2.9b) [in which $\kappa_m, \mathscr{H}_m = \operatorname{Ran} I^{(m)}$, $m = 1,...,n$, and $G(\alpha)$ are given] is $E(\alpha) = 0$ for $\alpha > 0$, and $I^{(m)} = 0$, $m = 1,...,n$.

We remark that Lemma 2.3 will be crucial for the construction, and there is no analog of it if the Hilbert problems are formulated for vector-valued solutions rather than operator-valued ones.

3. CONSTRUCTION WITH BOUND STATES

Let us now pose $H_n^1(S_x)$ for the family of S matrices S_x corresponding to shifted potentials, i.e., with $x \in \mathbb{R}^3$,

$$S_x(k;\theta,\theta') = S(k;\theta,\theta')e^{ikx\cdot(\theta-\theta')}. \tag{3.1}$$

As a result of this x dependence $\mathscr{H}_m^x$ will depend on x (see Sec. 4 of III) and so will $\Pi_x(k)$, but not κ_m. We define

$$\Omega_x(\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{-ik\alpha}[\Pi_x(k) - \mathbb{1}]$$

which is explicitly given by (4.7) of III for $\alpha < 0$, while $\Omega_x(\alpha) = 0$ for $\alpha > 0$. Then (2.7) leads to the relation for $\alpha > 0$

$$E_x(\alpha) = E_x^{\text{red}}(\alpha) + \int_{\alpha}^{\infty} d\beta\, \Omega_x(\alpha-\beta)E_x^{\text{red}}(\beta) \tag{3.2}$$

and for $\alpha < 0$

$$E_x(\alpha) = \Omega_x(\alpha) + \int_0^{\infty} d\beta\, \Omega_x(\alpha-\beta)E_x^{\text{red}}(\beta) \tag{3.2'}$$

in which E_x is related to F_x and E_x^{red} to F_x^{red} by (2.8).

Let us suppose now that for all x the operators $\mathscr{G}_x^{\text{red}}$ and $\mathscr{G}_x^{\text{red}\prime}$ are compact, neither has the eigenvalue 1, and that $G_x^{\text{red}} \in SL^2(\mathbb{R})$, so that $H_n^1(S_x)$ has a unique solution constructable via Lemma 2.2 by (2.3"). As a result E_x solves the system (2.9). Define

$$\Gamma_x(\alpha) = \left(\Delta - 2\frac{\partial}{\partial\alpha}\theta\cdot\nabla\right)E_x(\alpha), \tag{3.3}$$

where θ is regarded as a multiplicative operator. Application of the operator $\Delta - 2\partial/\partial\alpha\theta\cdot\nabla$ to (2.9) leads to the system

$$\Gamma_x(\alpha) = Q\Gamma_x(-\alpha)Q + G_x(\alpha)Q\mathscr{V}_x + \int_{-\infty}^{\infty} d\beta\, G_x(\alpha+\beta)\Gamma_x(\beta)Q \tag{3.4a}$$

and for $\alpha < 0$

$$\Gamma_x(\alpha) = i\sum_1^n \bar{I}_x^{(m)} e^{\alpha\kappa_m}, \tag{3.4b}$$

where, by (3.2) and (3.2')

$$\begin{aligned}\mathscr{V}_x &= 2\theta\cdot\nabla[E_x(0-) - E_x(0+)]\\ &= -2\theta\cdot\nabla[E_x^{\text{red}}(0+) - \Omega_x(0-)],\end{aligned} \tag{3.5}$$

and

$$\bar{I}_x^{(m)} = (\Delta - 2\kappa_m\theta\cdot\nabla)I_x^{(m)}. \tag{3.6}$$

[The derivation of (3.4a) uses the fact that

$$\left(\Delta - 2\frac{\partial}{\partial\alpha}\theta\cdot\nabla\right)G_x(\alpha) = G_x(\alpha)\left(\Delta + 2\frac{\partial}{\partial\alpha}\theta\cdot\nabla\right),$$

an integration by parts, and that (2.9a) implies $Q\mathscr{V}_xQ = \mathscr{V}_x$ if $G_x(\alpha)$ is continuous at $\alpha = 0$.] Multiplying (2.9a) by $\mathscr{V}_x$ on the right and subtracting (3.4a) we obtain

$$\hat{\Gamma}_x(\alpha) = Q\hat{\Gamma}_x(-\alpha)Q + \int_{-\infty}^{\infty} d\beta\, G_x(\alpha+\beta)\hat{\Gamma}_x(\beta)Q, \tag{3.7a}$$

where

$$\hat{\Gamma}_x(\alpha) = \Gamma_x(\alpha) - E_x(\alpha)\mathscr{V}_x, \tag{3.8}$$

and similarly from (2.9b) and (3.4b) for $\alpha < 0$

$$\hat{\Gamma}_x(\alpha) = i\sum_1^n \hat{I}_x^{(m)} e^{\alpha\kappa_m}, \tag{3.7b}$$

with

$$\hat{I}_x^{(m)} = \bar{I}_x^{(m)} - I_x^{(m)}\mathscr{V}_x. \tag{3.9}$$

Having solved $H_n^1(S_x)$ we know $I_x^{(m)}$ and hence the ranges of $\hat{I}_x^{(m)}$, $m = 1,...,n$. Lemma 2.3 then implies that the only solution of the system (3.7) is $\hat{\Gamma}_x = \hat{I}_x^{(m)} = 0$. Multiplying these equations by[4] $\hat{1}$ we obtain in detail for $\alpha < 0$ and $\alpha > 0$

$$\left(\Delta - 2\frac{\partial}{\partial\alpha}\theta\cdot\nabla\right)\eta_x(\theta,\alpha) = \int d\theta''\, \mathscr{V}_x(\theta'')E_x(\alpha,\theta,\theta''), \tag{3.10}$$

$$(\Delta - 2\kappa_m\theta\cdot\nabla)\eta_x^{(m)}(\theta) = \int d\theta''\, \mathscr{V}_x(\theta'')I_x^{(m)}(\theta,\theta''), \tag{3.11}$$

where

$$\eta_x(\theta,\alpha) = \int d\theta'\, E_x(\alpha,\theta,\theta'),$$

$$\eta_x^{(m)}(\theta) = \int d\theta'\, I_x^{(m)}(\theta,\theta'),$$

$$\mathscr{V}_x(\theta) = \int d\theta' \mathscr{V}_x(\theta,\theta')$$
$$= -2\theta\cdot\nabla[\eta_x^{\text{red}}(\theta,0+) - \Omega_x(\theta)],$$
$$\Omega_x(\theta) = \int d\theta' \Omega_x(0-,\theta,\theta'),$$

and $\mathscr{V}_x(\theta,\theta'), E_x(\alpha,\theta,\theta'), I_x^{(m)}(\theta,\theta')$, and $\Omega_x(\alpha,\theta,\theta')$ are the kernels of the operators $\mathscr{V}_x, E_x(\alpha), I_x^{(m)}$, and $\Omega_x(\alpha)$, respectively.

Suppose now that the *miracle* occurs i.e., that $\mathscr{V}_x(\theta)$ is independent of θ. We then define

$$V(x) = \mathscr{V}_x(\theta) = -2\theta\cdot\nabla[\eta_x^{\text{red}}(\theta,0+) - \Omega_x(\theta)]. \tag{3.12}$$

Then (3.10) and (3.11) become for $\alpha < 0$ and $\alpha > 0$

$$\left[\Delta - 2\frac{\partial}{\partial\alpha}\theta\cdot\nabla - V(x)\right]\eta_x(\alpha,\theta) = 0, \tag{3.13}$$

$$[\Delta - 2\kappa_m\theta\cdot\nabla - V(x)]\eta_x^{(m)}(\theta) = 0. \tag{3.14}$$

Furthermore

$$\gamma_x(k) = F_x(k)\hat{1}$$

satisfies the equation

$$\gamma_x(-k) = S_x^\dagger(k)Q\gamma_x(k) \tag{3.15}$$

obtained from (2.1) by multiplication by $\hat{1}$. Equation (3.13) implies that $\psi(k;\theta,x) = \gamma_x(k,\theta)\exp(ik\theta\cdot x)$ satisfies the Schrödinger equation. That it has the correct asymptotic form, with the function $A(k;\theta,\theta')$ as its scattering amplitude, is shown as (3.19) of III was derived. Eq. (3.15) shows that it obeys the required relation between incoming and outgoing wave solutions.

The constructed function $\psi(k;\theta,x)$ is meromorphic as a function of k in $\mathbb{C}^+$, with simple poles at $k = i\kappa_m$, $m = 1,\ldots,n$, and its residues there are

$$e^{-\kappa_m\theta\cdot x}\eta_x^{(m)}(\theta) = \sum_b Y_{\kappa_m}^b(-\theta)u_m^b(x)$$

because the range of $I_x^{(m)}$ is spanned by $Y_\kappa^b(-\theta)e^{-\kappa_m\theta\cdot x}$ (see Sec. 4 of III and Sec. 5 of II). If $V(x)$ has the needed regularity [say, (2.1) of II] then it follows that each $u_m^b(x)$, is in $L^2(\mathbb{R}^3)$, and (3.14) shows that, since the characters $Y_{\kappa_m}^b$, $b = 1,\ldots,N_m$, are linearly independent, each $u_m^b(x)$ is a bound-state eigenfunction of the Schrödinger equation with $V(x)$. Comparison with (5.8) of II shows that the functions $u_m^b(x)$ are linearly independent and have the asymptotic form (5.5) of II.

We have therefore proved the generalization of Theorem 3.1 of III to the case with bound states.

Theorem 3.1. Suppose a given unitary $S(k) = \mathbb{1} - (k/2\pi i)A(k)$ satisfies the Levinson theorem appropriate to N bound states [(5.3) of II] and that $A(k;\theta,\theta)$ is the boundary value of a meromorphic function with n simple poles. Construct the N_m characters, $m = 1,\ldots,n$, $\Sigma N_m = N$, as in Sec. 5 of II, and Π_x as in Sec. 4 of III, S_x by means of (3.1), and S_x^{red} by (2.5) from S_x. Suppose that the resulting $A_x^{\text{red}} = (2\pi i/k)(S_x^{\text{red}} - \mathbb{1}) \in \mathscr{A}$ [where $\mathscr{A}$ is the class defined in Sec. 3 of III; however, we have to add the condition that $G_x(\alpha;\theta,\theta')$ be continuous at $\alpha = 0$]. Then the equation

$$\eta_x^{\text{red}}(\alpha) = G_x^{\text{red}}(\alpha)\hat{1} + \int_0^\infty d\beta\, G^{\text{red}}(\alpha+\beta)\eta_x^{\text{red}}(\beta),$$

(in which G_x^{red} is constructed from A_x^{red} as in Lemma 2.1) has a unique solution $\eta_x^{\text{red}} \in L^2(\mathbb{R}_+ \times S^2)$. Suppose further that these solutions are *miraculous* in the sense that (3.12) is independent of θ. Construct η_x from η_x^{red} by (4.8) and (4.8') of III [i.e., (3.2) and (3.2') multiplied by $\hat{1}$] and define

$$\psi(k;\theta,x) = e^{ik\theta\cdot x} + \int_{-\infty}^{\infty} d\alpha\,\eta_x(\alpha,\theta)e^{ik(\alpha+\theta\cdot x)}$$

and

$$\psi^{(m)}(\theta,x) = \eta_x^{(m)}(\theta)e^{-\kappa_m\theta\cdot x}.$$

Then $\psi(k;\theta,x)$ and $\psi^{(m)}(\theta,x)$ satisfy the Schrödinger equations

$$[\Delta + k^2 - V(x)]\psi(k;\theta,x) = 0,$$
$$[\Delta - \kappa_m^2 - V(x)]\psi^{(m)}(\theta,x) = 0,$$

where $V(x)$ is given by (3.12). Furthermore, the outgoing and incoming wave solutions are connected by

$$\psi(-k;\theta,x) = \int d\theta' S^*(k;-\theta,\theta')\psi(k;\theta',x)$$

and the asymptotic form of $\psi(k;\theta,x)$ is given by (3.19) of III. If $V(x)$ satisfies (2.1) of III then $\psi^{(m)}(\theta,x)$ is of the form

$$\psi^{(m)}(\theta,x) = \sum_{b=1}^{N_m} Y_{\kappa_m}^b(-\theta)u_m^b(x),$$

where the N_m functions $u_m^b(x)$, $b = 1,\ldots,N_m$, are linearly independent bound-state eigenfunctions in $L^2(\mathbb{R}^3)$ of the Schrödinger equation with $V(x)$ and $\exists c$ such that[4]

$$\lim_{|x|\to\infty} e^{\kappa_m|x|}|x|u_m^b(x) = cY_{\kappa_m}^b(\hat{x}).$$

This theorem characterizes the "admissible" scattering amplitudes, but it does not give a sufficient condition for the existence of an underlying potential in a particular class of functions. While it is not hard to show that if kA (for fixed θ and θ') is absolutely integrable as a function of k and three times differentiable as a function of θ' then $V(x)$ decreases as $|x|^{-2}$ at infinity, it will require much more work to prove sufficient conditions for the potential to be $L^1(\mathbb{R}^3)$ or in the Rollnik class.

As a second remark we note that if the potential satisfies the hypotheses of Lemma 2.1 of II [the crucial one of which presumably is that $V \in L^1(\mathbb{R}^3)$] then by (3.8) of II the large-k behavior of $A(k;\theta,\theta')$ is dominated by a function $f(\tau)$ of $\tau = k(\theta - \theta')$. For such a function the integral

$$\int d\theta \int_0^\infty dk\, k^2|f(\tau)|^2 = \int d\theta\, |\theta - \theta'|^{-3} \times \int_0^\infty dt\, t^2|f(t\hat{\xi})|^2,$$

where $\hat{\xi} = (\theta - \theta')/|\theta - \theta'|$, is *always* divergent. Consequently, if[7] $\|kA(k)\|_2 \in L^2(\mathbb{R})$ then the associated potential cannot satisfy all the hypotheses of Lemma 2.1 of II; presumably it cannot be in $L^1(\mathbb{R}^3)$. It is therefore important to start with an amplitude such that $kA^{\text{red}} \in SL^2(\mathbb{R})$ as stated in the definitions of class $\mathscr{A}$ (Sec. 3 of III) but such that $\|kA\|_2 \notin L^2(\mathbb{R})$.[8]

An interesting point that emerges in the construction is that the analyticity of the forward amplitude (or of its trace) in $\mathbb{C}^+$ was never used in the inversion procedure, except to obtain the bound-state eigenvalues and characters. For this connection between bound states and scattering data to exist the potential has to be in L^1, and indeed, as Sec. 5 of II shows, more and more further restrictions on V have to be imposed if there are bound states of high multiplicity. It is not known what would happen if construction were attempted with an amplitude whose trace is not the boundary value of an analytic function holomorphic in $\mathbb{C}^+$, and with bound-state data that are independent of the scattering data. A plausible conjecture is that if the miracle occurs, a potential will emerge but it will not be in L^1. The alternative, that in such a case the miracle could not occur, would imply a quite surprising connection between the nature of solutions of the generalized Marchenko equations and analyticity of the trace of the amplitude.

4. THE JOST FUNCTION

Suppose an S matrix $S(k)$ is given and it satisfies the Levinson theorem [see Sec. 5 of II] for n bound states of degeneraries N_m, $m = 1,...,n$. We then find the bound-state eigenvalues κ_m, $m = 1,...,n$, and the characters $Y^b_{\kappa_m}(\theta)$ as shown in Sec. 5 of II. Let $Y^b_{\kappa_m}(-\theta)$, $b = 1,...,N_m$ span $\mathscr{H}_m$. We now pose the Hilbert problem $H^1_n(S)$ as stated and solved in Sec. 2. If the solution of this problem is $F(k)$ then we define the Jost function by

$$J(k) = [F(k)]^{-1}. \tag{4.1}$$

According to (2.7) correspondingly

$$J(k) = J^{\text{red}}(k)\widetilde{\Pi}(-k), \tag{4.2}$$

where $J^{\text{red}} = (F^{\text{red}})^{-1}$, and hence the operator $J(i\kappa_m)$ has a nullspace equal to $\mathscr{H}_m$, which includes the space spanned by the residue of $\psi(k;\theta,x)$ at its pole at $k = i\kappa_m$ for all values of x. The only question is whether $[F(k)]^{-1}$ has any singularities in $\mathbb{C}^+$. It follows from Lemma 2.1 that the Jost functions $J(k)$ satisfies the relation

$$J(-k) = QJ(k)QS(k) \tag{4.3}$$

and that it is *holomorphic* in $\mathbb{C}^+$. We state the result in the form of

Theorem 4.1. If the scattering amplitude $A(k,\theta,\theta')$ satisfies the hypotheses of Lemma 2.2 and neither $\mathscr{G}^{\text{red}}$ nor $\mathscr{G}^{\text{red}\prime}$ has the eigenvalues ± 1 then the Jost function $J(k)$ is given by (4.1) in terms of the unique solution of the Hilbert problem $H^1_n(S)$, $J^+ - \mathbb{1}$ is in $SL^2(\mathbb{R})$, and $J(k)$ is the boundary value of an analytic function $J(k)$, $\mathbb{C}^+ \to \mathscr{B}$, holomorphic in $\mathbb{C}^+$ such that for $\operatorname{Im} k > 0$

$$\lim_{|k|\to\infty} \|J(k) - \mathbb{1}\| = 0.$$

Furthermore, $J(k)$ is singular at $k = i\kappa_m$, $m = 1,...,n$, in the sense that $J(i\kappa_m)$ has a nontrivial null space equal to $\mathscr{H}_m$.

We note that Lemma 2.1 of III gives sufficient conditions on the potential for $\mathscr{G}^{\text{red}}$ and $\mathscr{G}^{\text{red}\prime}$ to be compact and for $\mathscr{G}^{\text{red}}$ to be in $SL^2(\mathbb{R})$.

For later purposes we will require certain properties of the expansion coefficients of the Jost function on the basis of the spherical harmonics. For the latter (normalized) we shall use the simplified notation $Y_L(\theta)$, in which capital L denotes the pair (l,m), $l = 0,1,2,...$, $-l \leqslant m \leqslant l$. As a preliminary we start by defining expansion coefficients of the wave function $\psi(k;\theta,x)$ as a function of θ. (We emphasize that *no* assumption is made that the potential is spherically symmetric.) Define

$$\psi_L(k,x) = \int d\theta\, Y^*_L(\theta)\psi(k;\theta,x), \tag{4.4}$$

which exists for all k and x if V satisfies (2.1) of II. It follows from the integral equation (2.3) of II and the expansion of the plane wave[4]

$$\psi^0(k;\theta,x) = e^{ik\theta\cdot x} = 4\pi \sum_L i^l j_l(k|x|)Y_L(\theta)Y^*_L(\hat{x}), \tag{4.5}$$

where $j_l(z)$ is a spherical Bessel function, that

$$\psi_L(k,x) = 4\pi i^l j_l(k|x|)Y^*_l(\hat{x}) - \frac{1}{4\pi}\int d^3y\, \frac{e^{ik|x-y|}}{|x-y|} V(y)\psi_L(k,y).$$

This equation can be solved by Fredholm methods analogous to those used in Sec. 2 of II. Since

$$|j_l(z)| \leqslant C_l \frac{|z|^l}{(1+|z|)^{l+1}} \tag{4.6}$$

one easily finds that if $D(0) \neq 0$, where $D(k)$ is the modified Fredholm determinant [(2.18) of II], and if V is such that

$$\int d^3x\, |V(x)|\, |x|^l < \infty \tag{4.7}$$

then as $k \to 0$

$$\psi_L(k,x) = O(k^l). \tag{4.8}$$

If V is such that $\exists \epsilon > 0$ for which

$$\int d^3x\, |V(x)|e^{\epsilon|x|} < \infty \tag{4.9}$$

then (4.7) holds for all l, and hence so does (4.8). What is more, one readily proves that if (4.9) holds then $\psi_L(k,x)$ and $\psi(k;\theta,x)$ are *analytic functions* of k for real $k \neq 0$, and including $k = 0$ if $D(0) \neq 0$. More precisely than (4.8) one can prove that for each L $\exists C$ such that

$$\| |V(x)|^{1/2}\psi_L(k,x)\| < C_l |k|^l, \tag{4.10}$$

where $\|\cdot\|$ denotes the $L^2(\mathbb{R}^3)$ norm.

As a next step we define similar expansion coefficients for the scattering amplitude in its dependence on θ and θ':

$$A_{LL'}(k) = \int d\theta\, d\theta'\, Y_L(\theta)Y^*_{L'}(\theta')A(k;\theta,\theta'). \tag{4.11}$$

It follows from formula (3.1) of II for the scattering amplitude that

$$A_{LL'}(k) = -(-i)^l \int d^3x\, V(x)Y^*_L(\hat{x})j_l(k|x|)\psi_{L'}(k,x). \tag{4.12}$$

One then easily proves by means of (4.6) and (4.10)

Lemma 4.2: If the potential satisfies (2.1) of II and (4.9) for some $\epsilon > 0$ and if $k = 0$ is not an exceptional point, then for all L and L', $A_{LL'}(k)$, as a function of k, is analytic on the real axis and $\exists C_{ll'}$ such that

$$|A_{LL'}(k)| < C_{ll'}|k|^{l+l'} \tag{4.13}$$

for all real k.

We note that in the spherically symmetric case $A_{LL'} = 0$ unless $L = L'$, and then (4.13) is a well-known result for exponentially decreasing potentials.

Corollary: On the assumptions of Lemma 4.2

$$\frac{\partial^n}{\partial k^n} A_{LL'}(k)|_{k=0} = 0 \quad \text{for } n < l + l'. \tag{4.14}$$

We now translate these results to the Fourier transform of kA, the function $G(\alpha;\theta,\theta')$ defined in (2.1). If we define

$$G_{LL'}(\alpha) = \int d\theta d\theta' Y_L(\theta) Y^*_{L'}(\theta') G(\alpha;\theta,\theta') = \frac{-i(-1)^l}{(2\pi)^2} \int_{-\infty}^{\infty} dk\, k e^{ik\alpha} A_{L'L}{}^*(k)$$

and

$$\rho^n_{LL'} = \frac{1}{n!} \int_{-\infty}^{\infty} d\alpha\, \alpha^n G_{LL'}(\alpha),$$

then (4.14) immediately implies

Lemma 4.3: On the assumptions of Lemma 4.2,

$$\rho^n_{LL'} = 0 \text{ for all } n \leqslant l + l'. \tag{4.15}$$

We now return to the Jost function and define

$$\mathfrak{L}(k) = \tilde{J}(k) - 1 \tag{4.16}$$

and

$$\mathfrak{L}_{LL'}(k) = \int d\theta\, d\theta'\, Y_L(\theta) Y^*_{L'}(\theta') \mathfrak{L}(k;\theta,\theta') \tag{4.17}$$

as well as the Fourier transforms

$$\mathscr{L}(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{-ik\alpha} \mathfrak{L}(k), \tag{4.18}$$

$$\mathscr{L}_{LL'}(\alpha) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{-ik\alpha} \mathfrak{L}_{LL'}(k). \tag{4.19}$$

We translate (4.3) into the equation

$$\mathscr{L}(\alpha)Q - Q\mathscr{L}(-\alpha) = G(-\alpha) + \int_{-\infty}^{\infty} d\beta\, G(-\alpha-\beta)\mathscr{L}(\beta). \tag{4.20}$$

Expansion on the spherical harmonics yields

$$(-1)^l \mathscr{L}_{L'L}(\alpha) - (-1)^{l'} \mathscr{L}_{L'L}(-\alpha) = G_{L'L}(-\alpha) + \sum_{L''} \int_{-\infty}^{\infty} d\beta\, G_{L'L''}(-\alpha-\beta) \mathscr{L}_{L''L}(\beta).$$

Multiplying by α^n and integrating we obtain

$$[(-1)^{l+n} - (-1)^{l'}]\Gamma^n_{L'L} = \rho^n_{L'L} + \sum_{l''=0}^{n-l'-1} \sum_{m''=-l''}^{l''} \sum_{s=0}^{n-l'-l''-1} \rho^{n-s}_{L'L''}\Gamma^s_{L''L} \tag{4.21}$$

by shifting variables of integration, using the binomial theorem, and defining

$$\Gamma^n_{L'L} = \frac{1}{n!} \int_{-\infty}^{\infty} d\alpha\, \alpha^n \mathscr{L}_{L'L}(\alpha). \tag{4.22}$$

The upper limits on the sums in (4.21) originate from (4.15). For each fixed n and L, (4.21) constitutes a finite set of equations for $\Gamma^s_{L'L}$ with $s \leqslant n$ and $l' \leqslant n$. Define $\mathscr{M}_l$ to be the set of all $\Gamma^n_{L'L}$ with $l' + n < l$. For $\Gamma^n_{L'L} \in \mathscr{M}_l$ (4.21) reduces to the following sets of homogeneous equations: For $0 \leqslant r \leqslant \min(2l', l-1)$, r even,

$$\sum_{l''=0}^{l-1-r} \sum_{m'=-l''}^{l''} \sum_{s=0}^{l-l''-1-r} \rho^{l+l'-r-s}_{L'L''}\Gamma^s_{L''L} = 0; \tag{4.23a}$$

for $l' + 1 \leqslant n \leqslant l - l'$,

$$[(-1)^{l+n} - (-1)^{l'}]\Gamma^n_{L'L} = \sum_{l''=0}^{n-l'-1} \sum_{m''=-l''}^{l''} \sum_{s=0}^{n-l'-l''-1} \rho^{n-s}_{L'L''}\Gamma^s_{L''L}; \tag{4.23b}$$

and for $n < \min(l - l', l' + 1)$, $l + l' + n$ odd,

$$\Gamma^n_{L'L} = 0. \tag{4.23c}$$

For a fixed value of l, l' may be allowed to run from 0 to ∞ in (4.23a). Therefore (4.23a) make up an infinite set of homogeneous equations for the (finite number of) members of $\mathscr{M}_l$. The set of ρ's that would allow them to have nontrivial solutions is at most *exceptional*. In the generic case we may conclude that (4.15) and (4.20) imply that

$$\Gamma^n_{L'L} = 0 \quad \text{for } n < l - l'. \tag{4.24}$$

We note parenthetically that for $n \geqslant l + l'$, with $r = n - l - l'$, for $r > 0$ even, (4.21) becomes

$$\sum_{l''=0}^{l-1+r} \sum_{m''=-l''}^{l''} \sum_{s=0}^{l-l''-1+r} \rho^{l+l'+r-s}_{L'L''}\Gamma^s_{L''L} = -\rho^{l+l'+r}_{L'L},$$

which for fixed r and l is an infinite set of inhomogeneous equations for the finite set of $\Gamma^s_{L''L}$. This implies that unless the set of ρ's is, again, exceptional, no solution for $\Gamma^s_{L''L} \notin \mathscr{M}_l$ exists. It follows that *in general* Eq. (4.13), with an $S(k)$ that is analytic at $k = 0$, will have no solution that is analytic there. Thus not even (4.9) assures analyticity of $J(k)$ at $k = 0$.

From (4.24) and the inversion of (4.19) we conclude

Lemma 4.4: If $A(k)$ is such that (4.13) holds, then every solution of (4.3) is such that near $k = 0$

$$\mathfrak{L}_{L'L}(k) = O(k^n), \tag{4.25}$$

where $n = \max(0, l - l')$. [Here $\mathfrak{L}_{LL'}$ is defined by (4.16) and (4.17) in terms of the solution $J(k)$ of (4.3).]

Consider now

$$\mathfrak{L}_L(k,\theta) = \int d\theta'\, Y^*_L(\theta')\mathfrak{L}(k;\theta,\theta') \tag{4.26}$$

and calculate

$$\int d\theta\, \mathfrak{L}_L(k,\theta) e^{ik\theta\cdot x} = 4\pi \sum_{L'<L} \mathfrak{L}_{L'L}(k) i^{l'} Y^*_{L'}(\hat{x}) j_{l'}(k|x|) + \int d\theta\, \mathfrak{L}_L(k,\theta) E_L(k,\theta,x), \tag{4.27}$$

where

$$E_L(k,\theta,x) = e^{ik\theta\cdot x} - 4\pi \sum_{L'<L} i^{l'} Y_{L'}(\theta) Y^*_{L'}(\hat{x}) j_{l'}(k|x|).$$

It follows from (4.25) and (4.26) that the sum on the right of (4.27) is $O[(|x|k)^l]$ as $k \to 0$. It is easily seen from (4.6) and the analyticity of E_L that $E_L = O[(|x|k)^{l+1}]$. Since by Theorem

4.1, $L(k)\in SL^2(\mathbb{R})$, it follows that

$$\int_{-\infty}^{\infty} dk \int d\theta\, |\mathfrak{L}_L(k,\theta)|^2 < \infty,$$

which implies that

$$\lim_{k\to 0} k^2 \int d\theta\, |\mathfrak{L}_L(k,\theta)|^2 = 0.$$

As a result the integral in (4.27) is $O[(|x|k)^l]$ and therefore, as $k\to 0$

$$\int d\theta\, \mathfrak{L}_L(k,\theta) e^{ik\theta\cdot x} = O\,[(|x|k)^l]. \tag{4.28}$$

5. THE REGULAR SOLUTION

As in II we define the regular solution of the Schrödinger equation by[9]

$$\phi = J\psi \tag{5.1}$$

or more explicitly,

$$\phi(k;\theta,x) = \int d\theta'\, J(k;\theta,\theta')\psi(k;\theta',x). \tag{5.1'}$$

It therefore satisfies the integral equation

$$\phi(k;\theta,x) = e^{ik\theta\cdot x} + \int d\theta'\, \mathfrak{L}(k;\theta',\theta) e^{ik\theta'\cdot x} - \frac{1}{4\pi}\int d^3y\, \frac{e^{ik|x-y|}}{|x-y|} V(y)\phi(k;\theta,y).$$

Its spherical-harmonic projection

$$\phi_L(k,x) = \int d\theta\, Y_L^*(\theta)\phi(k;\theta,x)$$

consequently solves

$$\phi_L(k,x) = 4\pi i^l j_l(k|x|)Y_L^*(x) + \int d\theta\, \mathfrak{L}_L(k,\theta)e^{ik\theta\cdot x} - \frac{1}{4\pi}\int d^3y\, \frac{e^{ik|x-y|}}{|x-y|} V(y)\phi_L(k,y).$$

By (4.6) and (4.28) the inhomogeneity here is $O\,[(|x|k)^l]$ as $k\to 0$. It then easily follows that if $k=0$ is not exceptional, and if V satisfies (4.9) then

$$\phi_L(k,x) = O(k^l). \tag{5.2}$$

It follows from (5.1), (4.3), and (3.16') of II, and the unitarity of S that

$$\phi(-k;\theta,x) = \phi(k;-\theta,x). \tag{5.3}$$

This, together with the analyticity of $J\psi$ in $\mathbb{C}^+$, implies that ϕ is an entire analytic function of k (for all x and almost all θ). It can thus be expanded in a convergent power series in k:

$$\phi(k;\theta,x) = \sum_{n=0}^{\infty} k^n C_n(\theta,x) \tag{5.4}$$

whose coefficients C_n are functions of θ and x. The result (5.2) then implies that *in general*

$$\int d\theta \left.\frac{\partial^n \phi(k;\theta,x)}{\partial k^n}\right|_{k=0} Y_L(\theta) = 0 \tag{5.5}$$

for all $l>n$. The words "in general" are intended to say that we have not been able to rule out the possibility that if the scattering amplitude is *exceptional* (5.5) may fail.

The result (5.5) is well known for central potentials. Eq. (8.5) shows that in that case $\phi_L(k,x)$ differs from the regular radial function $\phi_l(k,|x|)$ by a factor of k^l, and ϕ_l is known to be entire analytic. However, in order to prove this, and hence (5.5), in the case of a central potential no requirement as strong as (4.9) is needed. Since $\phi_l(k,|x|)$ can be defined directly by means of a boundary condition, its analyticity can be proved by means of its Volterra equation. In the noncentral case no such direct definition of $\phi_L(k,x)$ is known and (5.5) has had to be proved by the circuitous route of Sec. 4, via the intermediary of the scattering amplitude's property (4.13). This property requires, in the central case too, the exponential decay (4.9) of the potential.

Note that since $Y_L(-\theta) = (-1)^l Y_L(\theta)$, the definition of $\phi_L(k,x)$ shows that it may be written in the form

$$\phi_L(k,x) = k^l \hat{\phi}_L(k^2,x),$$

where $\hat{\phi}_L$ is an entire analytic function of k^2. Now we may choose such linear combinations of $Y_l^m(\theta)$ to form $Y_L(\theta)$ that $k^l Y_L(\theta)$ is a homogeneous polynomial of degree l in the three Cartesian components of the vector $k\theta = (k_1,k_2,k_3)$. It follows therefore from (5.2) that $\phi(k;\theta,x)$ is an entire analytic function of each of the Cartesian components of $k\theta$ separately.

Let us look at the integrability of ϕ as a function of k on the real line. Let a be in $L^2(S^2)$. Then by (5.1)

$$(a,(\phi-\psi^0)) = (a,(J-\mathbb{1})(\psi-\psi^0)) + (a,(J-\mathbb{1})\psi^0) + (a(,\psi-\psi^0)),$$

where ψ^0 is defined by (4.5). Since by Theorem 4.1 $(J^+ - \mathbb{1}) \in SL^2(S^2)$, by Lemma 2.4 of II, and since ψ^0 is uniformly bounded, each of the three terms on the right-hand side is square integrable as a function of k. Therefore for each fixed $a\in L^2(S^2)$

$$\int dk\, |(a,(\phi(k,x) - \psi^0(k,x))|^2 < \infty \tag{5.6}$$

the inner product being in $L^2(S^2)$. This may be stated by saying that, as a function of k, $\phi-\psi^0$ is weakly square integrable: $(\phi-\psi^0)\in WL^2(\mathbb{R})$.

We also note that it follows from (5.1), Theorem 4.1, Lemma 2.3 of II, and Lemma 2.4 of II, that for any fixed $a\in L^2(S^2)$ the function $(a,\phi)(k)$ is an entire function of exponential order $|x|$. We shall summarize all of these results in

Theorem 5.1: Suppose that V satisfies the hypotheses of Lemma 2.1 of II, of Lemma 2.4 of II, and of Theorem 4.1. Then there exists a "regular solution" $\phi(k;\theta,x)$ of the Schrödinger equation in $\mathbb{R}^3$ given by (5.1) with the following properties:

(a) ϕ satisfies the symmetry (5.3);

(b) as a function of k, $(\phi-\psi^0)\in WL^2(\mathbb{R})$,

where ψ_0 is a defined by (4.5), $\phi-\psi^0$ is regarded as a function $\mathbb{R}\to L^2(S^2)$, and $WL^2(\mathbb{R})$ is defined by (5.6);

(c) for all fixed x and almost all fixed θ, $\phi(k;\theta,x)$ is an entire analytic function of k, and for each fixed $a\in L^2(S^2)$, (a,ϕ) is of exponential order $|x|$.

If furthermore, V satisfies (4.12) for some $\epsilon>0$, then

(d) *in general* each expansion coefficient of ϕ as a function of θ on the basis of the spherical harmonics satisfies (5.2) near 0, or equivalently, ϕ satisfies (5.5);

(e) under these conditions ϕ is an entire analytic function of each Cartesian component of $k\theta$ separately.

The meaning of "in general" is explained below (5.5) and below (4.23c).

6. THE GENERALIZED GL EQUATION

As in (5.1) of III we define the Fourier transform of $\phi - \psi^0$ in its dependence upon k

$$q(x,\theta,\alpha) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{-ik\alpha}[\psi^0(k;\theta,x) - \phi(k;\theta,x)], \tag{6.1}$$

where ψ^0 is defined by (4.5). This Fourier integral exists for almost all θ and α (and all x) in the WL^2 sense, by Theorem 5.1, so that for each x, and each $a \in L^2(S^2)$, $\int d\theta\, a^*(\theta)\, q(x,\theta,\alpha) \in L^2(\mathbb{R})$. Furthermore, (5.5) implies that for all n and all $l > n$

$$\int d\alpha \int d\theta\, \alpha^n q(x,\theta,\alpha) Y_L(\theta) = 0, \tag{6.2}$$

and (5.3), that

$$q(x,-\theta,-\alpha) = q(x,\theta,\alpha). \tag{6.3}$$

It follows from (6.2) and (6.3) that $q(x,\theta,\alpha)$ is a *Radon transform*. If we define the three-dimensional Fourier transform

$$\check{h}(x,y) = (1/2\pi)^3 \int_0^{\infty} dk\, k^2 \int d\theta \times e^{-ik\theta\cdot y}[\psi^0(k;\theta,x) - \phi(k;\theta,x)] \tag{6.4}$$

then q is the Radon transform of $\check{h}$,

$$q(x,\theta,\alpha) = \int d^3y\, \delta(\alpha - \theta\cdot y)\check{h}(x,y). \tag{6.5}$$

Since there is no assurance that $(\psi_0 - \phi) \in L^2(\mathbb{R}^3)$, $\check{h}$, as a function of y, is generally not square integrable and may be a distribution.

It follows from (c) of Theorem 5.1 and the Paley–Wiener theorem[10] that for every $a \in L^2(S^2)$ the function of α

$$\int d\theta\, a^*(\theta) q(x,\theta,\alpha)$$

has support in the interval $(-|x|,|x|)$:

$$\phi(k;\theta,x) = \psi^0(k;\theta,x) - \int_{-|x|}^{|x|} d\alpha\, e^{ik\alpha} q(x;\theta,\alpha) \tag{6.6}$$

in the weak L^2 sense. It then follows[11] from (6.2) that the support of $\check{h}(x,y)$ is in the ball $|y| \leqslant |x|$. [Alternatively, this conclusion may be reached by combining (c) and (e) of Theorem 5.1 and using the Paley–Wiener theorem for each of the three Fourier integrals with respect to the three Cartesian components of $k\theta$.] This establishes the "triangularity" of $\check{h}(x,y)$ that had been assumed in II on insufficient grounds.

The generalized GL procedure may now be based entirely on $\check{h}(x,y)$, or else on $q(x,\theta,\alpha)$. The former is very much simpler and more elegant, but it has the drawback of dealing with kernels that may be distributions. The arguments of II, Secs. 7 and 8, lead to the generalized GL equation for $|x| \geqslant |y|$,

$$\check{h}(x,y) = \check{h}_0(x,y) - \int_{|z|<|x|} d^3z\, \check{h}(x,z)\check{h}_0(z,y), \tag{6.7}$$

which is (8.4) of II. The kernel $\check{h}_0(z,y)$ is given by

$$\check{h}_0(z,y) = \int \psi^0(k,z)\, d(\rho - \rho^0)\, \psi^0(k,y)^*, \tag{6.8}$$

which is more explicitly written out below (8.5) of II, but where in our present notation

$$M(k) = Q\,[J(k)J^\dagger(k)]^{-1}Q - 1. \tag{6.9}$$

The partial differential equations satisfied by $\check{h}$, and representations of the potential, are given in Sec. 5 of III.

One may also obtain an equation for q by taking a *partial* Radon transform of (6.7) [since (6.7) holds only for $|y| < |x|$]. Defining

$$\int_{|y|<|x|} d^3y\, \check{h}_0(z,y)\delta(\alpha - \theta\cdot y) = q^0_{|x|}(z,\theta,\alpha),$$

we find from (6.7) for $|\alpha| < |x|$

$$q(x,\theta,\alpha) = q^0_{|x|}(x,\theta,\alpha) - \int_{|z|<|x|} d^3z\, \check{h}(x,z) q^0_{|x|}(z,\theta,\alpha).$$

Furthermore, since q^0 can be written in the form

$$q^0_{|x|}(z,\theta,\alpha) = \int d\theta'\, \mathscr{U}_{|x|}(\theta',\theta'\cdot z;\theta,\alpha),$$

and

$$\int d^3z\, \check{h}(x,y) f(\theta\cdot z) = \int d\beta\, q(x,\theta,\beta) f(\beta),$$

we obtain the generalized GL equation for $q(x,\theta,\alpha)$, for $|\alpha| < |x|$,

$$q(x,\theta,\alpha) = \int d\theta'\, \mathscr{U}_{|x|}(\theta',\theta'\cdot x;\theta,\alpha) - \int d\theta' \int_{-|x|}^{|x|} d\beta\, q(x,\theta',\beta)\mathscr{U}_{|x|}(\theta',\beta;\theta,\alpha), \tag{6.10}$$

which replaces (8.3) of II.[12]

The partial Radon transform $\mathscr{U}_x$ is calculated by means of the formula (for $\alpha \leqslant |x|$)

$$\begin{aligned}\mathscr{J}(k,\theta\cdot\theta',|x|,\alpha) &= \int_{|y|<|x|} d^3y\, \delta(\alpha - \theta\cdot y) e^{ik\theta'\cdot y} \\ &= \frac{2\pi(|x|^2 - \alpha^2)^{1/2}}{k\,|\theta\times\theta'|} e^{ik\alpha\theta\cdot\theta'} \times J_1[k(|x|^2 - \alpha^2)^{1/2}|\theta\times\theta'|],\end{aligned}$$

where $|\theta\times\theta'| = [1 - (\theta\cdot\theta')^2]^{1/2}$ and J_1 is the Bessel function of order one. Thus

$$\begin{aligned}\mathscr{U}_{|x|}(\theta',\beta;\theta,\alpha) = (2\pi)^{-3}\int_0^{\infty} dk\, k^2 \int d\theta'' &\times e^{ik\beta}\mathscr{J}(k,\theta\cdot\theta'',|x|,\alpha) M(k,\theta',-\theta'') \\ &+ \sum_{n=1}^{l} \int d\theta''\, e^{-\kappa_n\beta} M_{\kappa_n}(\theta',\theta'') \\ &\times \mathscr{J}(i\kappa_n,\theta\cdot\theta'',|x|,\alpha),\end{aligned} \tag{6.11}$$

where M and M_{κ_n} are the kernels, defined in (8.1) and (5.22) of II, that enter the spectral function.

7. OTHER GENERALIZED GL EQUATIONS

We shall derive a generalization of the GL equation that leads from a given "reference potential" to another potential, and a generalization of the nonlinear GL equation.

Let us write Eq. (7.8″) of II in the form

$$\phi^{V}(k) = \omega^{V0}\phi^{0}(k)$$

and

$$\phi^{W}(k) = \omega^{W0}\phi^{0}(k) = \omega^{W0}(\omega^{V0})^{-1}\phi^{V}(k),$$

so that if

$$\phi^{W}(k) = \omega^{WV}\phi^{V}(k)$$

then

$$\omega^{W0}(\omega^{V0})^{-1} = \omega^{WV}.$$

It follows that $\omega^{WV} = (\omega^{VW})^{-1}$ and hence

$$\omega^{WV} = \omega^{W0}\omega^{0V}. \tag{7.1}$$

Writing $\omega = \mathbb{1} - \check{h}$ we therefore have

$$\check{h}^{WV} = \check{h}^{W0} + \check{h}^{0V} - \check{h}^{W0}\check{h}^{0V}$$

or, since $\check{l}^{V0} = -\check{h}^{0V}$, if we write $\omega^{-1} = \mathbb{1} + \check{l}$,

$$\check{h}^{WV} = \check{h}^{W0} - \check{l}^{V0} + \check{h}^{W0}\check{l}^{V0}. \tag{7.2}$$

Now, $\check{h}^{W0}(x,y) = 0$ for $|y| > |x|$, and hence $\check{l}^{W0}(x,y) = 0$ for $|y| > |x|$. Consequently (7.2) reads explicitly

$$\check{h}^{WV}(x,y) = \check{h}^{W0}(x,y) - \check{l}^{V0}(x,y) + \int_{|y|<|z|<|x|} d^3z\, \check{h}^{W0}(x,z)\check{l}^{V0}(z,y)$$

and implies that $\check{h}^{WV}(x,y) = 0$ for $|y| > |x|$, and hence $\check{l}^{WV} = 0$ for $|y| > |x|$.

The completeness for W reads, symbolically,

$$\delta = \int \phi^{W} d\rho^{W} \phi^{W\dagger} = \omega^{WV} \int \phi^{V} d\rho^{W} \phi^{V\dagger} (\omega^{WV})^{\dagger} \tag{7.3}$$

or

$$[(\omega^{WV})^{\dagger}]^{-1} = \omega^{WV} \int \phi^{V} d\rho^{W} \phi^{V\dagger},$$

whereas the completeness for V reads

$$\delta = \int \phi^{V} d\rho^{V} \phi^{V\dagger} \tag{7.4}$$

so that

$$\omega^{WV} = \omega^{WV} \int \phi^{V} d\rho^{V} \phi^{V\dagger}$$

and therefore

$$[(\omega^{WV})^{\dagger}]^{-1} - \omega^{WV} = \omega^{WV} \int \phi^{V} d(\rho^{W} - \rho^{V}) \phi^{V\dagger}. \tag{7.5}$$

If we write explicitly

$$\check{h}^{W}_{V}(x,y) = \int \phi^{V}(k,x)\, d\,[\rho^{W}(k) - \rho^{V}(k)]\phi^{V}(k,y)^{\dagger} \tag{7.6}$$

then (7.2) implies that for $|y| < |x|$

$$\check{h}^{WV}(x,y) = \check{h}^{W}_{V}(x,y) - \int_{|z|<|x|} d^3z\, \check{h}^{WV}(x,z)\check{h}^{W}_{V}(z,y). \tag{7.7}$$

The solution of the Schrödinger equation with the potential W is given by

$$\phi^{W}(k,\theta,x) = \phi^{V}(k,\theta,x) - \int d^3y\, \check{h}^{WV}(x,y)\phi^{V}(k,\theta,y), \tag{7.8}$$

from which we obtain the equation

$$[\Delta_x - \Delta_y - W(x) + V(y)]\check{h}^{WV}(x,y) = \delta^3(x-y)[V(x) - W(x)]. \tag{7.9}$$

Thus,

$$V(u) - W(u) = -2 \lim_{\epsilon\to 0} \epsilon^2 \int_{\theta\cdot u>0} d\theta \times \theta\cdot\nabla_u \check{h}(u + \tfrac{1}{2}\epsilon\theta, u - \tfrac{1}{2}\epsilon\theta). \tag{7.10}$$

The generalized nonlinear GL equation is obtained similarly by concluding from (7.3) that

$$(\omega^{WV})^{-1}[(\omega^{WV})^{\dagger}]^{-1} = \int \phi^{V} d\rho^{W} \phi^{V\dagger}$$

and subtracting (7.4),

$$\omega^{VW}(\omega^{VW})^{\dagger} - \delta = \int \phi^{V} d(\rho^{W} - \rho^{V}) \phi^{V\dagger}.$$

Explicitly, this reads, for $|x| > |y|$,

$$\check{h}^{VW}(x,y) = \check{h}^{W}_{V}(x,y) - \int_{|z|<|y|} d^3z\, \check{h}^{VW}(x,z)\check{h}^{VW}(y,z)^{*}. \tag{7.11}$$

It must be noted, however, that if $\check{h}$ is a distribution this equation may not make any sense.

8. CENTRAL POTENTIALS

Suppose that $V(x) = V(|x|)$. In that case $\check{h}(x,y)$ can depend on $\hat{x}$ and $\hat{y}$ only via $\hat{x}\cdot\hat{y}$ and we expand

$$|x||y|\check{h}(x,y) = \sum_{L} Y_L(\hat{x})Y^{*}_{L}(\hat{y})K_l(|x|,|y|), \tag{8.1}$$

Eq. (5.7″) of III then becomes for $s < t$

$$\left[\frac{\partial^2}{\partial s^2} - \frac{\partial^2}{\partial t^2} + l(l+1)\left(\frac{1}{t^2} - \frac{1}{s^2}\right) + V(t)\right]K_L(t,s) = 0 \tag{8.2}$$

and $K(t,s) = 0$ for $s > t$. Eq. (5.9) of III implies that for all l

$$-2\frac{\partial}{\partial s}K_l(s,s) = V(s). \tag{8.3}$$

Alternatively, if we wish to regard $K_l(t,s)$ as satisfying a partial differential equation even across its discontinuity at $t = s$ then this equation is

$$\left[\frac{\partial^2}{\partial s^2} - \frac{\partial^2}{\partial t^2} + l(l+1)\left(\frac{1}{t^2} - \frac{1}{s^2}\right) + V(t)\right]K_l(t,s) = -2\delta(t-s)\frac{d}{ds}K_l(s,s), \tag{8.4}$$

which in view of (8.3), is identical with the result of inserting (8.1) in (5.7) of III.

We define the functions $\phi_l(k,s)$ and $\phi^{0}_{l}(k,s)$ by the expansions

$$\phi(k,\theta,s) = \sum_L \frac{(ik)^l}{|x|(2l+1)!!} \phi_l(k,|x|) Y_L^*(\theta) Y_L(\hat{x}), \quad (8.5)$$

$$e^{ik\theta\cdot x} = \sum_L \frac{(ik)^l}{|x|(2l+1)!!} \phi_l^0(k,|x|) Y_L^*(\theta) Y_L(\hat{x}). \quad (8.5')$$

Then (5.5′) of III leads to

$$\phi_l(k,t) = \phi_l^0(k,t) - \int_0^t ds_1\, K_l(t,s) \phi_l^{(0)}(k,s). \quad (8.6)$$

The generalized Gel'fand–Levitan equation (6.7) is easily seen to lead to

$$K_l(t,s) = g_l(t,s) - \int_0^t du\, K_l(t,u) g_l(u,s), \quad (8.7)$$

where g_l is defined by the expansion

$$|x||y|\check{h}_0(x,y) = \sum_L Y_L(\hat{x}) Y_L^*(\hat{y}) g_l(|x|,|y|)[(2l+1)!!]^{-2} \quad (8.8)$$

so that

$$g_l(t,s) = \int \phi_l^0(k,s) d(\rho_l - \rho_l^0) \phi_l^0(k,t), \quad (8.9)$$

where $d(\rho_l - \rho_l^0)$ is defined by the expansion

$$d(\rho - \rho^0)(k,\theta,\theta') = \sum_L Y_L(\theta) Y_L^*(\theta') d(\rho_l - \rho_l^0)(k). \quad (8.10)$$

Equations (8.3), (8.2), and (8.7) are the well-known equations[13] for the inverse problem of angular momentum l.

We also note that the relation (5.1′) together with the expansions

$$\psi(k,\theta,x) = (1/k|x|) \sum_L i^l \psi_l(k,|x|) Y_L^*(\theta) Y_L(\hat{x}), \quad (8.11)$$

$$J(k,\theta,\theta') = \sum_L f_l(k) Y_L(\theta) Y_L^*(\theta'), \quad (8.12)$$

and (8.5) lead to

$$\phi_l(k,|x|) = (2l+1)!! k^{-l-1} f_l(k) \psi_l(k,|x|). \quad (8.13)$$

From this we may conclude[14] that f_l is the well-known Jost function for the angular momentum l. Equation (8.12) may be replaced by

$$J(k,\theta,\theta') - \delta(\theta,\theta') = (1/4\pi) \sum_l (2l+1) \times [f_l(k) - 1] P_l(\theta\cdot\theta'). \quad (8.12')$$

Thus the three-dimensional equations reduce to all the well-known ones for central potentials. The question whether $\check{h}$ and J are *functions* rather than distributions is related to the question of the convergence of the expansions in (8.1) and (8.12′). A similar reduction of the generalized Marchenko equation for central potentials does not appear to be possible. This is not surprising in view of the fact that the radial Marchenko equations deal with Jost solutions.

9. SUMMARY

Let us refer to the mapping of a potential V as a function $\mathbb{R}^3 \to \mathbb{R}$ (with varying restrictions needed for various purposes) to the scattering amplitude A as a function $\mathbb{R} \times S^2 \times S^2 \to \mathbb{C}$, defined by the Schrödinger equation, as $\mathscr{F}$. The series of papers II, III, and the present one, have dealt with its inverse, $\mathscr{F}^{-1}$, leading from A to V. The following aspects of $\mathscr{F}^{-1}$ have been considered:

(1) Reconstruction,
  (a) uniqueness,
  (b) reconstruction procedure;

(2) Construction,
  (a) existence,
  (b) uniqueness,
  (c) construction procedure.

By (1) I mean the reconstruction of the underlying potential if the given scattering amplitude is known to be associated with one. The uniqueness questions (1a) and (2b) are answered by Lemma 3.1 of II (which is not new). Two alternative new reconstruction procedures have been given: a generalized Marchenko equation and a generalized Gel'fand–Levitan equation.

If there are no bound states [which can be ascertained from the scattering amplitude by means of the Levinson theorem, (5.3) of II] then the reconstruction proceeds via the generalized Marchenko equations, a linear integral equation whose kernel was proved to be compact (Theorem 2.1 of III). If there are bound states then their eigenvalues and characters (which here take the place of the norming constants in one dimension) are constructed from A by a method given in Sec. 5 of II. The reconstruction via a generalized Marchenko equation is then accomplished by Sec. 4 (Lemma 4.1) of III.

In the generalized GL method it is first necessary to construct the generalized Jost function from the given amplitude. This is done via Theorem 4.1 of this paper by solving a generalized Hilbert problem by means of a generalized Marchenko equation (Lemma 2.2 of this paper). This leads to the spectral function, (7.13) of II [(6.9) of this paper], for the "regular solutions." For potentials with exponential fall-off generalized linear and nonlinear GL equations are established "in general" in Secs. 6 and 7 of this paper. In contrast to the generalized Marchenko equation they can by expected to have noncompact kernels that are distributions. On the other hand, they are integral equations on finite domains. Reduction of the generalized GL equation for central potentials to the well-known radial GL equations is given in Sec. 8 of this paper.

If an amplitude A, $\mathbb{R} \times S^2 \times S^2 \to \mathbb{C}$, is given and is not known to be associated with a potential, there is a nontrivial existence or *characterization* problem: to characterize those functions A that are in the range of $\mathscr{F}$. A partial answer is provided by the construction procedure, as given by Theorem 3.1 of III if there are no bound states, and by Theorem 3.1 of the present paper if there are. The essential characterizing property is the *miracle*, as defined in these theorems. However, the problem of characterizing the functions whose pre-images under $\mathscr{F}$ are potentials in certain specific relevant classes, such as $L^1 \cap L^2$ or the Rollnik class, is still open.[15]

The following new results have emerged as incidental effects of the solutions of the inverse problem. The bound states of the Schrödinger equation in $\mathbb{R}^3$ have received a new characterization (Sec. 5 of II); a set of generalized Hilbert problems for operator-valued functions has been solved (Sec. 2 of this paper); a Jost function and a "regular solution" of the Schrödinger equation in $\mathbb{R}^3$ have been constructed and their most important properties have been established (Secs. 4 and 5 of this paper).

Note added in proof: I am indebted to Professor Y. Saitō for pointing out to me that the equation four lines from the bottom of the left-hand column of p. 1713 of II is in error and should be replaced by

$$V'(x,y,\theta) = \frac{(\theta - \hat{y}\theta\cdot\hat{y})\cdot\nabla V(x+y)}{1-(\theta\cdot\hat{y})^2}.$$

As a result the proof of Lemma 3.2 of II is invalid. A modification of this proof by means of Hölder's inequality leads to the following replacement of Lemma 3.2: If the assumptions stated in Lemma 3.2 of II are made, and in addition it is assumed that $\exists C_1$, and μ such that for all $k\in\mathbb{R}^3$

$$|\widetilde{V}(k)| \leqslant C_1(\mu^2 + |k|^2)^{-1},$$

where $\widetilde{V}$ is the Fourier transform of V, then for all $p > 4$, $\exists C_2$ such that for all $f\in L^p(S^2)$

$$\int_{-\infty}^{\infty} dk\, k^2 \|A_k f\|_p^2 < C\|f\|_p^2,$$

where $\|\cdot\|_p$ is the L_p-norm.

This form of Lemma 3.2 (and its corresponding change in the corollary stated in II) suffices for all subsequent results.

I am also aware of some misprints in III. The lower limits on the k-integrals in the equations on lines 7 to 10 from the bottom of the right-hand column on p. 2192 should all be $-\infty$. Equation (A3) is valid for $0 < \alpha < 1$. The equation four lines below (A3) should read

$$(\theta' - \theta'')^2(\theta - \theta'')^2 = (2 - |\theta + \theta'|u)^2 - |\theta - \theta'|^2(1-u^2)\cos^2\phi,$$

and similarly in the integral in the next line. In line 6 from below in the same column, it should be $O(|a^2 - 1|^{\alpha/2 - 1})$, and in line 4 from below, $a^2 \geqslant b^2$.

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[1] R. G. Newton, J. Math. Phys. **21**, 1698 (1980) and **22**, 631 (1981); these papers will be referred to as II.

[2] R. G. Newton, J. Math. Phys. **22**, 2191 (1981); this paper will be referred to as III.

[3] See Sec. 5 of III. Some of the contents of Sec. 6 and all of Secs. 7 and 8 were already contained in the preprint of III, but they were omitted from the published version as the generalized GL equation then lacked foundation.

[4] A reminder of our notation: † stands for the adjoint, * for the operator whose kernel is the complex conjugate, $\sim$ for the operator whose kernel is the transpose; Q is the operator with the property $(Q,f)(\theta) = f(-\theta)$ for $f\in L^2(S^2)$; and $SL^2(\mathbb{R})$ is the class of functions $\mathbb{R}\to\mathscr{B}$ that are square integrable in the strong sense, as defined in the Corollary to Lemma 3.2 of II. $\hat{1}$ denotes the function in $L^2(S^2)$, $\hat{1}(\theta)\equiv 1$; $\hat{x}$ denotes the unit vector in $\mathbb{R}^3$, $\hat{x} = x/|x|$.

[5] $\mathbb{C}^{\pm}$ are the open upper and lower halves of the complex plane, respectively.

[6] Ran stands for the range of the operator.

[7] By $\|\cdot\|_2$ we mean the Hilbert-Schmidt norm on $L^2(S^2)$.

[8] Equation (3.12) may be used to obtain a representation of the potential that is the generalization of (4.11) of II with $D = 1$ for no bound states. However, note that the right-hand side of (4.11) of II should be multiplied by 2, because of the discontinuity of $\eta(\alpha)$ at $\alpha = 0$. I am indebted to Dr. L. Trlifaj for pointing this out.

[9] As noted in III we are no longer using a notation in which operators act to the left. Therefore, (5.1) is (7.1) of II, but our present J corresponds to $\widetilde{J}$ there.

[10] See, for example, K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer, New York, 1977), p. 36.

[11] D. Ludwig, Commun. Pure and Appl. Math. **19**, 49 (1966); Theorem 4.9, p. 69.

[12] Equation (8.3) of II, which was obtained by taking a full Radon transform, is incorrect, and so is (8.7) of II, which is based upon it.

[13] See, for example, R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), pp. 614 and 615, Eqs. (20.6), (20.9), and (20.8).

[14] See Ref. 13, p. 374.

[15] The fact that the characterizations of amplitudes in the range of $\mathscr{F}$ require the solutions of an integral equation and is not possible directly, means that the three-dimensional inverse problem treated here, is not well posed. Most small perturbations of a given admissible amplitude lead to functions that are inadmissible, and we do not know how to make admissible perturbations. Thus the inversion is not stable.

Maximum of the spin-flip cross section from unitarity and three constraints [a)]

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A sharper upper bound on the spin-flip cross section is found by applying the variational calculus with three equality constraints and unitarity. These are the total cross section, elastic cross section, and the forward slope. Unitarity of the partial waves provides the inequality constraints.

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I. INTRODUCTION

In two previous papers[1,2] we extended the application of the variational calculus to problems in elementary particle scattering[3,4] to cases with spin. The results of Ref. 1 on the upper bound of the spin-flip cross section were applied to $\pi^+ p$ scattering to find numerical solutions.[5] We are in the process of applying these results to other spin $\frac{1}{2}$–spin 0 cases. The solutions we found show that the bound gets weaker as the energy increases.

It can even be larger than the elastic cross section. Considering that the input is the total cross section, the result is still an improvement on the input. At low energies there is no difference between the elastic and total cross sections. However, at large energies, adding the elastic cross section as a third constraint should improve the bound.

In this paper we add the elastic cross section to our constraints. The results are not altogether trivial. With two constraints the inelastic class I^+I^- had no contribution. Now it may contribute. Partially inelastic classes I^+B^- and I^-B^+ could contribute before only to saddle points, but not to the maximum. With three constraints they can contribute to the upper bound.

In Sec. II we write the expressions for the spin-flip cross section, total cross section, elastic cross section, and the forward slope. Using these quantities, as well as the partial waves, we write the Lagrange function. The maximum conditions are found by taking the second derivatives of this function. In this section we also define four classes according to the elasticity of the partial waves.

In Sec. III the forms of the partial waves in these four classes are found. Because of the existence of the third constraint the possibilities are larger and the expressions a little more complicated. The existence of the third l-independent Lagrange parameter γ makes it possible for the maximum conditions to be satisfied in all classes. As we already mentioned before, this was not the case with two constraints.

In conclusion we summarize and discuss our results.

II. CONSTRAINTS, LAGRANGE FUNCTION, AND THE FOUR CLASSES

For simplicity we define G, A_0, E, and S instead of σ_{SF}, σ^T, σ^E, and $dA/dt\,|_{t=0}$.

$$G = \frac{k^2}{2\pi}\sigma_{SF} = \sum \frac{2l(l+1)}{2l+1}[(a_{l+} - a_{l-})^2 + (r_{l+} - r_{l-})^2], \tag{1}$$

$$A_0 = \frac{k^2}{4\pi}\sigma^T = \sum[(l+1)a_{l+} + la_{l-}], \tag{2}$$

$$E = \frac{k^2}{4\pi}\sigma^E = \sum[(l+1)(a_{l+}{}^2 + r_{l+}{}^2) + l(a_{l-}{}^2 + r_{l-}{}^2)], \tag{3}$$

$$S = 4k^2\frac{k}{(s)^{1/2}}\frac{dA}{dt}\bigg|_{t=0} \sum l(l+1)[(l+1)a_{l+} + la_{l-}]. \tag{4}$$

Here σ_{SF} is the spin-flip cross section, σ^T the total cross section, σ^E elastic cross section, A the imaginary part of the scattering amplitude, $dA/dt\,|_{t=0}$ the forward slope, k the c.m. momentum, and $a_{l+}, a_{l-}, r_{l+}, r_{l-}$ the imaginary and real parts of the partial waves.

The inequality constraints of unitarity are

$$u_l = a_{l+} - a_{l+}^2 - r_{l+}^2 \geqslant 0, \tag{5}$$

$$v_l = a_{l-} - a_{l-}^2 - r_{l-}^2 \geqslant 0. \tag{6}$$

The problem is to maximize G subject to constraints (2)–(6). The Lagrange function is

$$L = G + \alpha A_0 + \gamma E + \beta S + \sum(l+1)\lambda_l u_l + \sum l\mu_l v_l. \tag{7}$$

To preserve notation of the previous work we called the Lagrange parameter of the new constraint E, γ. As before, $\lambda_l \geqslant 0$, $\mu_l \geqslant 0$ from the theory of inequality constraints and the factors $(l+1)$ and l are chosen for convenience. We also define the frequently appearing combinations

$$B \equiv \frac{2l}{2l+1}, \quad D \equiv \frac{2(l+1)}{2l+1}. \tag{8}$$

We now differentiate L with respect to a_{l+}, a_{l-}, r_{l+} and r_{l-}.

$\dfrac{\partial L}{\partial a_{l+}} = 0$ gives

$$(B + \gamma - \lambda_l)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + \lambda_l] = 0. \tag{9}$$

$\dfrac{\partial L}{\partial a_{l-}} = 0$ gives

$$Da_{l+} - (D + \gamma - \mu_l)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + \mu_l] = 0. \tag{10}$$

$\dfrac{\partial L}{\partial r_{l+}} = 0$ gives

$$(B + \gamma - \lambda_l)r_{l+} - Br_{l-} = 0. \tag{11}$$

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$$\frac{\partial L}{\partial r_{l-}} = 0 \text{ gives}$$

$$Dr_{l+} - (D+\gamma-\mu_l)r_{l-} = 0. \tag{12}$$

As in the case with two constraints we define four classes according to whether a pair of amplitudes f_{l+}, f_{l-} are both elastic, both inelastic, first one elastic and second inelastic, and vice versa:

$$I^+I^- = \{l\,|u_l>0, v_l>0\}, \quad \lambda_l = 0, \mu_l = 0, \tag{13}$$

$$I^+B^- = \{l\,|u_l>0, v_l=0\}, \quad \lambda_l = 0, \mu_l \geqslant 0, \tag{14}$$

$$I^-B^+ = \{l\,|u_l=0, v_l>0\}, \quad \lambda_l \geqslant 0, \mu_l = 0, \tag{15}$$

$$B^+B^- = \{l\,|u_l=0, v_l=0\}, \quad \lambda_l \geqslant 0, \mu_l \geqslant 0. \tag{16}$$

For a fixed value of l a pair of amplitudes f_{l+}, f_{l-} belongs to one and only one of these classes.

To find the maximum conditions we also take the second derivatives of L,

$$\frac{\partial^2 L}{\partial a_{l+}^2} = (B+\gamma-\lambda_l)2(l+1), \tag{17}$$

$$\frac{\partial^2 L}{\partial a_{l+}\partial a_{l-}} = -BD(2l+1), \tag{18}$$

$$\frac{\partial^2 L}{\partial r_{l+}^2} = 2(l+1)(B+\gamma-\lambda_l), \tag{19}$$

$$\frac{\partial^2 L}{\partial r_{l+}\partial r_{l-}} = -BD(2l+1), \tag{20}$$

$$\frac{\partial^2 L}{\partial a_{l-}^2} = 2l(D+\gamma-\mu_l), \tag{21}$$

$$\frac{\partial^2 L}{\partial r_{l-}^2} = 2l(D+\gamma-\mu_l). \tag{22}$$

For a maximum we have from the negativeness of the second variations

$$B+\gamma-\lambda_l \leqslant 0, \tag{23}$$

$$D+\gamma-\mu_l \leqslant 0. \tag{24}$$

III. FORMS OF THE PARTIAL WAVES IN DIFFERENT CLASSES

Class I^+I^-: In this class $\lambda_l = 0, \mu_l = 0$. Hence Eqs. (9) and (10) become

$$(B+\gamma)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta] = 0, \tag{25}$$

$$Da_{l+} - (D+\gamma)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta] = 0. \tag{26}$$

Unless $2+\gamma=0$, we have (27)

$$a_{l+} = a_{l-} = -\frac{1}{2\gamma}[\alpha + l(l+1)\beta]. \tag{28}$$

From unitarity

$$0 \leqslant -\frac{1}{2\gamma}[\alpha + l(l+1)\beta] \leqslant 1. \tag{29}$$

From maximum conditions (23) and (24) we find for this class

$$B+\gamma \leqslant 0, \tag{30}$$

$$D+\gamma \leqslant 0. \tag{31}$$

Since γ is l independent only partial waves with l values that satisfy (30) and (31) can contribute to the solution. We also note that in the absence of the constraint E this class did not contribute. Equations (11) and (12) become for this class

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{32}$$

$$Dr_{l+} - (D+\gamma)r_{l-} = 0. \tag{33}$$

r_{l+} and r_{l-} will satisfy these two equations only if the determinant vanishes. In this case

$$\gamma = -2. \tag{34}$$

We note that when the determinant of (32) and (33) vanishes, that is when $\gamma+2=0$, the inhomogeneous Eqs. (25) and (26) are consistent. That is,

$$\frac{B+\gamma}{D} = \frac{B}{D+\gamma} = -1 \tag{35}$$

is satisfied.

In this case the real and imaginary parts of the partial waves must satisfy

$$(B-2)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta] = 0, \tag{36}$$

$$(B-2)r_{l+} - Br_{l-} = 0, \tag{37}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 > 0, \tag{38}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 > 0. \tag{39}$$

When the determinant does not vanish

$$r_{l+} = r_{l-} = 0. \tag{40}$$

Class I^+B^-: In this class $\lambda_l = 0, \mu_l \geqslant 0$. Equations (9)–(12) become

$$(B+\gamma)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta] = 0, \tag{41}$$

$$Da_{l+} - (D+\gamma-\mu_l)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta + \mu_l] = 0, \tag{42}$$

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{43}$$

$$Dr_{l+} - (D+\gamma-\mu_l)r_{l-} = 0. \tag{44}$$

For r_{l+} and r_{l-} to be different from zero the determinant of Eqs. (43) and (44) must vanish. This condition gives

$$\mu_l(B+\gamma) = \gamma(\gamma+2). \tag{45}$$

This is an equation between γ and l. Since γ is l-independent only certain l values can satisfy this equation. When the determinant of Eqs. (43) and (44) vanishes the other two determinants in Eqs. (41) and (42) must also be zero; i.e.,

$$\frac{B+\gamma}{D} = \frac{B}{D+\gamma-\mu_l} = -\frac{\alpha + l(l+1)\beta}{\alpha + l(l+1)\beta + \mu_l}. \tag{46}$$

This equation gives either

$$\gamma + 2 = \mu_l = 0 \tag{47}$$

or

$$\alpha + l(l+1)\beta + \gamma = 0. \tag{48}$$

Since in the class I^+B^-, $\lambda_l = 0$, the first case is similar to the class I^+I^- except that $v_l = 0$. The second possibility $l(l+1) = -(\alpha+\gamma)/\beta$ can be satisfied at most by two l values and at most by one positive integer l value if α, β and γ are such that the right-hand side is a positive integer.

In the first case the equations satisfied by the partial waves are identical with Eqs. (36)–(39), except that (39) is now an equality.

In the second case they are

$$(B+\gamma)a_{l+} - Ba_{l-} - \tfrac{1}{2}\gamma = 0, \tag{49}$$

$$(B+\gamma)r_{l+} - Br_{l-} = 0, \tag{50}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 > 0, \tag{51}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 = 0. \tag{52}$$

When the determinant is different from zero

$$r_{l+} = r_{l-} = 0.$$

In this class $v_l = a_{l-} - a_{l-}^2 - r_{l-}^2 = 0$.

Except for the special values of l that might satisfy Eq. (45) we have in general

$$v_l = a_{l-} - a_{l-}^2 = 0.$$

Hence

$$a_{l-} = \begin{array}{l}\nearrow 1\\ \searrow 0\end{array}.$$

(i) If $a_{l-} = 1$, from Eq. (41) we find for a_{l+}

$$a_{l+} = \frac{1}{B+\gamma}\{B - \tfrac{1}{2}[\alpha + l(l+1)\beta]\}. \tag{53}$$

Equation (42) gives

$$\mu_l = \frac{2+\gamma}{B+\gamma}[\alpha + l(l+1)\beta + 2\gamma]. \tag{54}$$

We now impose the unitarity condition

$$0 \leqslant a_{l+} \leqslant 1$$

on Eq. (53). Together with the maximum condition (23) this gives

$$2B \leqslant \alpha + l(l+1)\beta \leqslant -2\gamma. \tag{55}$$

The maximum condition (24) imposed on (54), together with $\mu_l \geqslant 0$, Eq. (55), and $B+\gamma \leqslant 0$, gives

$$\gamma \geqslant -2 \tag{56}$$

and

$$\alpha + l(l+1)\beta \leqslant \frac{BD}{2+\gamma} - \gamma. \tag{57}$$

(ii) If $a_{l-} = 0$, we find from Eq. (41)

$$a_{l+} = -\frac{1}{2(B+\gamma)}[\alpha + l(l+1)\beta]. \tag{58}$$

From Eq. (42) we find

$$\mu_l = -\frac{2+\gamma}{B+\gamma}[\alpha + l(l+1)\beta]. \tag{59}$$

The unitarity condition

$$0 \leqslant a_{l+} \leqslant 1$$

imposed on (58) together with the maximum condition (23) gives

$$0 \leqslant \alpha + l(l+1)\beta \leqslant -2(B+\gamma). \tag{60}$$

The maximum condition (24) imposed on (59), together with

$$\mu_l \geqslant 0,$$

Eq. (60), and $B+\gamma \leqslant 0$ gives

$$\gamma + 2 \geqslant 0 \tag{61}$$

and

$$\alpha + l(l+1)\beta \geqslant -\frac{BD}{2+\gamma} - \gamma. \tag{62}$$

Unlike the two-constraint (A_0,S) case, we can not sum the contributions of partial waves we found to G, A_0, E, and S explicitly using the sums of powers of integers. This is because of the presence of γ next to B in the denominators of (53) and (58). However in applications to numerical problems there is no difficulty in forming finite series and we did not find much difference in using the closed form of the series or summing a finite series with a few terms.[5]

Class I^-B^+: In this class $\lambda_l \geqslant 0, \mu_l = 0$. Equations (9)–(12) become

$$(B+\gamma-\lambda_l)a_{l+} - Ba_{l-} + \tfrac{1}{2}[\alpha + l(l+1)\beta + \lambda_l] = 0, \tag{63}$$

$$Da_{l+} - (D+\gamma)a_{l-} - \tfrac{1}{2}[\alpha + l(l+1)\beta] = 0, \tag{64}$$

$$(B+\gamma-\lambda_l)r_{l+} - Br_{l-} = 0, \tag{65}$$

$$Dr_{l+} - (D+\gamma)r_{l-} = 0. \tag{66}$$

For r_{l+} and r_{l-} to be different from zero the determinant of Eqs. (65) and (66) must vanish. This condition gives

$$\lambda_l(D+\gamma) = \gamma(\gamma+2). \tag{67}$$

This is an equation in γ and l. Since γ is l independent only certain l values can satisfy this equation.

When the determinant of Eqs. (65) and (66) vanishes the other two determinants in Eqs. (63) and (64) must also be zero; i.e.,

$$\frac{B+\gamma-\lambda_l}{D} = \frac{B}{D+\gamma} = -\frac{\alpha + l(l+1)\beta + \lambda_l}{\alpha + l(l+1)\beta}. \tag{68}$$

This equation gives either

$$\gamma + 2 = \lambda_l = 0 \tag{69}$$

or

$$\alpha + l(l+1)\beta + \gamma = 0. \tag{70}$$

Since in the class I^-B^+, $\mu_l = 0$, the first case is similar to the class I^+I^- except that $u_l = 0$. Again, the second possibility (70) can be satisfied at most by two l values, and only by one positive integer l if $-(\alpha+\gamma)/\beta$ is a positive integer.

In the first case [Eq. (69)] the equations satisfied by the partial waves are identical with Eqs. (36)–(39), except that (38) is now an equality.

In the second case [Eq. (70)] they are

$$Da_{l+} - (D+\gamma)a_{l-} + \tfrac{1}{2}\gamma = 0, \tag{71}$$

$$Dr_{l+} - (D+\gamma)r_{l-} = 0, \tag{72}$$

$$a_{l+} - a_{l+}^2 - r_{l+}^2 = 0, \tag{73}$$

$$a_{l-} - a_{l-}^2 - r_{l-}^2 > 0. \tag{74}$$

When the determinant of (65) and (66) is different from zero

$$r_{l+} = r_{l-} = 0.$$

Except for the special values of l that might satisfy Eq. (67) we have in general

$$u_l = a_{l+} - a_{l+}^2 = 0.$$

Hence

$$a_{l+} = \begin{array}{l}\nearrow 1\\ \searrow 0\end{array}$$

(i) If $a_{l+}=1$, from Eq. (64) we find for a_{l-}

$$a_{l-}=\frac{1}{D+\gamma}\{D-\tfrac{1}{2}[\alpha+l(l+1)\beta]\}. \tag{75}$$

Equation (63) gives

$$\lambda_l=\frac{2+\gamma}{D+\gamma}[\alpha+l(l+1)\beta+2\gamma]. \tag{76}$$

We impose the unitarity condition

$$0\leqslant a_{l-}\leqslant 1$$

on Eq. (75). Together with the maximum condition (24) this gives

$$2D\leqslant\alpha+l(l+1)\beta\leqslant-2\gamma. \tag{77}$$

The maximum condition (23) imposed on (76), together with $\lambda_l\geqslant 0$, Eq. (77), and $D+\gamma\leqslant 0$ gives

$$\gamma\geqslant-2 \tag{78}$$

and

$$\alpha+l(l+1)\beta\leqslant\frac{BD}{2+\gamma}-\gamma. \tag{79}$$

(ii) If $a_{l+}=0$, from Eq. (64) we find for a_{l-}

$$a_{l-}=-\frac{1}{2(D+\gamma)}\{\alpha+l(l+1)\beta\}. \tag{80}$$

Equation (63) gives

$$\lambda_l=-\frac{2+\gamma}{D+\gamma}[\alpha+l(l+1)\beta]. \tag{81}$$

We impose the unitarity condition

$$0\leqslant a_{l-}\leqslant 1$$

on Eq. (80). Together with the maximum condition (24) this gives

$$0\leqslant\alpha+l(l+1)\beta\leqslant-2(D+\gamma). \tag{82}$$

The maximum condition (23) imposed on (81), together with $\lambda_l\geqslant 0$, Eq. (82), and $D+\gamma\leqslant 0$ gives

$$\gamma+2\geqslant 0 \tag{83}$$

and

$$\alpha+l(l+1)\beta\geqslant-\frac{BD}{2+\gamma}-\gamma. \tag{84}$$

The remarks about summing the series of G, A_0, E, and S with the partial waves given by their forms in the class I^+B^- apply also to the class I^-B^+

Class B^+B^-: In this class neither λ_l nor μ_l is zero. As before we have to solve Eqs. (9)–(12). We also note that the determinant of the homogeneous equations (11) and (12) is the same as the determinant of the inhomogeneous equations (9) and (10). If this determinant does not vanish the solutions of Eqs. (11) and (12) are trivial:

$$r_{l+}=0,\quad r_{l-}=0.$$

Since in the class B^+B^-, $u_l=0$ and $v_l=0$ we have

$$a_{l+}=\begin{smallmatrix}\nearrow 1\\ \searrow 0\end{smallmatrix}\quad\text{and}\quad a_{l-}=\begin{smallmatrix}\nearrow 1\\ \searrow 0\end{smallmatrix}.$$

This leads to four possibilities:

(i) When $a_{l+}=a_{l-}=0$,

$$\alpha+l(l+1)\beta+\lambda_l=0,\quad\alpha+l(l+1)\beta+\mu_l=0.$$

Hence

$$\lambda_l=-\{\alpha+l(l+1)\beta\}\geqslant 0,$$
$$\mu_l=-\{\alpha+l(l+1)\beta\}\geqslant 0. \tag{85}$$

Obviously this case does not contribute to G, A_0, E, or S.

(ii) When $a_{l+}=0$, $a_{l-}=1$, Eqs. (9) and (10) give

$$\lambda_l=2B-[\alpha+l(l+1)\beta]\geqslant 0, \tag{86}$$

$$\mu_l=2(D+\gamma)+[\alpha+l(l+1)\beta]\geqslant 0. \tag{87}$$

With Eqs. (23) and (24) we also find from (86) and (87)

$$\alpha+l(l+1)\beta+\gamma\leqslant B, \tag{86a}$$

$$\alpha+l(l+1)\beta+\gamma\geqslant-D. \tag{87a}$$

The analysis of these inequalities as functions of l is the same as in the two-constraint (A_0,S) case. $y=\alpha+l(l+1)\beta$ is a parabola in the variable l with its extremum at $l=-\frac{1}{2}$ The sign of β determines whether the extremum is a maximum or minimum. B and D, as defined by Eqs. (8), are respectively monotonically increasing or decreasing functions, asymptotically approaching 1.

(iii) When $a_{l+}=1$, $a_{l-}=0$, Eqs. (9) and (10) give

$$\lambda_l=2(B+\gamma)+[\alpha+l(l+1)\beta]\geqslant 0, \tag{88}$$

$$\mu_l=2D-[\alpha+l(l+1)\beta]\geqslant 0. \tag{89}$$

With Eqs. (23) and (24) we also find from (88) and (89)

$$\alpha+l(l+1)\beta+\gamma\geqslant-B, \tag{88a}$$

$$\alpha+l(l+1)\beta+\gamma\leqslant D. \tag{89a}$$

(iv) When $a_{l+}=1$, $a_{l-}=1$, Eqs. (9) and (10) give

$$\lambda_l=\mu_l=2\gamma+[\alpha+l(l+1)\beta]\geqslant 0. \tag{90}$$

With Eqs. (23) and (24) we also find from (90)

$$\alpha+l(l+1)\beta+\gamma\geqslant B, \tag{90a}$$

$$\alpha+l(l+1)\beta+\gamma\geqslant D. \tag{90b}$$

We note that this case does not contribute to G even though it contributes to A_0, E, and S.

(v) Finally there is a fifth case for the class B^+B^-. This is when the determinant of the homogeneous equations (11) and (12) vanishes. In this case the remaining two determinants of Eqs. (9) and (10) also must vanish. We can then write

$$\frac{B+\gamma-\lambda_l}{D}=\frac{B}{D+\gamma-\mu_l}=-\frac{\alpha+l(l+1)\beta+\lambda_l}{\alpha+l(l+1)\beta+\mu_l}. \tag{91}$$

These equations are satisfied for

$$\lambda_l=\mu_l=2+\gamma. \tag{92}$$

In this case Eq. (9) is proportional to (10) and Eq. (11) proportional to (12). The partial waves are given by the solutions of the following set:

$$Da_{l+}+Ba_{l-}-\tfrac{1}{2}[\alpha+l(l+1)\beta+2+\gamma]=0, \tag{93}$$

$$Dr_{l+}+Br_{l-}=0, \tag{94}$$

$$a_{l+}-a_{l+}^2-r_{l+}^2=0, \tag{95}$$

$$a_{l-}-a_{l-}^2-r_{l-}^2=0. \tag{96}$$

The solutions of these equations are

$$a_{l+} = \frac{1}{4}\frac{\alpha + l(l+1)\beta + \gamma + 2}{[\alpha + l(l+1)\beta + \gamma]D}[\alpha + l(l+1)\beta + \gamma + D - B], \tag{97}$$

$$a_{l-} = \frac{1}{4}\frac{\alpha + l(l+1)\beta + \gamma + 2}{[\alpha + l(l+1)\beta + \gamma]B}[\alpha + l(l+1)\beta + \gamma + B - D], \tag{98}$$

$$r_{l+}^2 = \frac{1}{16}\frac{\alpha + l(l+1)\beta + \gamma + 2}{[\alpha + l(l+1)\beta + \gamma]^2 D^2}[\alpha + l(l+1)\beta + \gamma + D - B][B^2 - (\alpha + l(l+1)\beta + \gamma - D)^2], \tag{99}$$

$$r_{l-}^2 = \frac{1}{16}\frac{\alpha + l(l+1)\beta + \gamma + 2}{[\alpha + l(l+1)\beta + \gamma]^2 B^2}[\alpha + l(l+1)\beta + \gamma + B - D][D^2 - (\alpha + l(l+1)\beta + \gamma - B)^2]. \tag{100}$$

Here because of the positivity of λ_l and μ_l and Eq. (92)

$$\gamma + 2 \geqslant 0.$$

Unitarity imposed on (97) and (98) give two possible domains both for a_{l+} and a_{l-}. They are

$$\frac{2}{2l+1} \leqslant \alpha + l(l+1)\beta + \gamma \leqslant 2, \tag{101}$$

$$-2 \leqslant \alpha + l(l+1)\beta + \gamma \leqslant -\frac{2}{2l+1}. \tag{102}$$

The contributions of a_{l+}, a_{l-}, r_{l+} and r_{l-} to A_0, S and G are given by

$$A_0 = \frac{1}{4}\sum_{L_1}^{L_2}[\alpha + l(l+1)\beta + \gamma + 2](2l+1)$$
$$= \frac{\alpha + \gamma + 2}{4}[(L_2+1)^2 - L_1^2] + \frac{\beta}{8}[L_2(L_2+1)^2(L_2+2) - (L_1-1)L_1^2(L_1+1), \tag{103}$$

$$S = \frac{1}{4}\sum_{L_1}^{L_2}[\alpha + l(l+1)\beta + \gamma + 2]l(l+1)(2l+1) = \frac{\alpha + \gamma + 2}{8}[L_2(L_2+1)^2(L_2+2) - (L_1-1)L_1^2(L_1+1)]$$
$$+ \frac{\beta}{12}[L_2^2(L_2+1)^2(L_2+2)^2 - (L_1-1)^2 L_1^2(L_1+1)^2], \tag{104}$$

$$G = \frac{1}{8}\sum_{L_1}^{L_2}\{4 - [\alpha + l(l+1)\beta + \gamma]^2\}(2l+1) = \frac{4 - (\alpha+\gamma)^2}{8}[(L_2+1)^2 - L_1^2] - \frac{(\alpha+\gamma)\beta}{8}$$
$$\times [L_2(L_2+1)^2(L_2+2) - (L_1-1)L_1^2(L_1+1)]$$
$$- \frac{\beta^2}{24}[L_2^2(L_2+1)^2(L_2+2)^2 - (L_1-1)^2 L_1^2(L_1+1)^2]. \tag{105}$$

Because in the class B^+B^- both partial waves are elastic, the contributions of the amplitudes (97)–(100) to E are equal to their contribution to A_0, that is Eq. (103),

$$E = \frac{1}{4}\sum_{L_1}^{L_2}(\alpha + l(l+1)\beta + \gamma + 2)(2l+1). \tag{106}$$

This completes the discussion of the forms of the partial waves in all classes.

Solutions are found by fitting A_0, E, and S with partial waves from different classes. Three Lagrange parameters α, β, and γ are determined by these three conditions. However, the choice of partial waves from different classes is not trivial and has to be made systematically. In general when A_0, E, and S are fitted the partial waves will have the required form, but will not satisfy the conditions [like (101) and (102) for instance] imposed by unitarity and maximality. These conditions have to be tested after the constraints are fitted. If solutions exist they will satisfy these conditions. Those partial waves that do not satisfy the required conditions have to be discarded. We refer the reader to Ref. 5 for the applications to π^+p, as well as the π^-p and KN cases that will be forthcoming.

IV. CONCLUSION

We applied the variational calculus in a systematic way to scattering problems with spin to extremize one quantity (in this case G) with other quantities as constraints (3 in this case). The unitarity of the partial waves is taken fully into account, treating the unitarity as inequality constraints. The single series form of G, A_0, E, and S in terms of real and imaginary parts of the partial waves is crucial for the approach used.

For the spin $\frac{1}{2}$–spin 0 particle scattering there are two partial waves f_{l+}, f_{l-} belonging to the same l values (except $l = 0$). This makes it possible to study all possibilities by considering four classes in which both partial waves are elastic, inelastic, one elastic the other inelastic, and vice versa. Since one or both of the l-dependent Lagrange parameters λ_l, μ_l vanish in some classes, the partial waves have well defined forms in each class. Moreover, the unitarity and the maximum condition put lower and upper limits on the quantity $\alpha + l(l+1)\beta$ that appears in partial waves.

Numerical solutions are found by fitting the given constraints with partial waves from different classes, which have the prescribed forms of each class and also satisfy the conditions imposed by unitarity and maximality. At high energies where A_0 and E differ appreciably three constraints should restrict G much better than two constraints.

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Building things in general relativity [a)]

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In the context of general relativity, there is a sense in which certain objects cannot be constructed, using reasonable matter, from normal initial conditions. An attempt is made to capture this sense as a definition. The implications of such a definition, along with some related results and open questions, are discussed.

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1. INTRODUCTION

Certain solutions of Einstein's equation in certain contexts are commonly regarded as unphysical,[1] on the grounds that they represent systems which could not be "built from ordinary matter and initial conditions." A prominent example is the solutions representing white holes.[2] Can one in fact pin down any precise sense in which it is actually true that certain objects cannot be built within general relativity?

A suitable definition might have direct application to such issues as cosmic censorship,[3] or the energy–entropy conjecture of Bekenstein.[4] But it could also have other ramifications. The solutions representing white holes, of course, manifest a number of surprising features peculiar to general relativity. What other unexpected features lie before us in the theory? It would seem to be difficult to find even a line of attack on so broad a question. Yet one line would be to search for other solutions satisfying the definition of "unbuildable." As a second example, one might hope to learn something by turning such a definition on other theories. Consider electromagnetism. No analogous notion seems to present itself naturally there, i.e., Maxwell's equations are normally taken as the sole conditions on the fields. Can this difference be traced, for instance, to some structural difference between the theories themselves?

We here provide some preliminary ideas and results on these issues.

A tentative definition can be formulated as follows. By an *initial-data set* we mean a three-dimensional manifold T with positive-definite metric q_{ab} and symmetric tensor field p_{ab}, such that the mass and momentum density of matter, given by the constraint equations

$$\mu = \tfrac{1}{2}(\mathscr{R} - p^{ab}p_{ab} + p^{m}{}_{m}{}^{2}), \quad J^a = D_b(p^{ab} - p^{m}{}_{m}q^{ab}), \tag{1}$$

satisfy the energy condition

$$\mu \geqslant (J^a J_a)^{1/2}, \tag{2}$$

where D_a is the derivative operator, and $\mathscr{R}$ the scalar curvature, of q_{ab}. Let $I = (T, q_{ab}, p_{ab})$ and $I' = (T', q'_{ab}, p'_{ab})$ be two such initial-data sets. Think of I as representing the "assembled building materials" and of I' as the "final configuration to be built". Accordingly, we say that I' can be *built* from I, $I \rightarrow I'$, if, given any compact subset C' of T', there exists a space-time with Cauchy surfaces S and S' such that (i) the induced data on S coincides with that of I, and the induced data on a compact subset of S' coincides with that of C' in I', (ii) S' is everywhere to the future of S, and (iii) the space-time satisfies the energy condition

$$T_{ab}t^a\hat{t}^b \geqslant 0 \tag{3}$$

for all future-directed timelike vectors t^a and $\hat{t}^b$, where T_{ab} is the stress-energy by Einstein's equation.

The restriction to a compact subset of S'—physically, the restriction to building only finite objects—is imposed to avoid some awkward issues involving boundary conditions. This restriction implies in particular that "can be built from" will in general be time-reversible in the appropriate sense. Note that this is not an initial-value formulation: Nothing playing the role of an equation of state has been specified. The manipulation of the stresses—which are entirely at our disposal—is the mechanism by which one would "build" I' from I. But this arrangement, we claim, is physically appropriate. After all, the process of building a log cabin, say, from a forest consists exactly of applying judiciously chosen stresses.

The idea would be to find a large class of initial-data sets—consisting of almost all—such that any in this class can be built from any other. These would represent the "reasonable initial conditions". The remaining initial-data sets would represent the "unbuildable objects" including, presumably, the holes, and perhaps various other configurations.

2. OTHER THEORIES

It is convenient, in order to gain a general idea of what this definition means and how it operates, to consider first some analogous, but simpler, arrangements.

Consider the theory of test stress-energies. An initial-data set I consists of fields μ and J^a *on Euclidean* 3-*space* T, subject to the energy condition (2). We write $I \rightarrow I'$ if, given any compact subset C' of T', there exists in Minkowski space-time a conserved stress-energy field T_{ab} satisfying the energy condition (3) and two parallel flat spacelike Cauchy surfaces, S' to the future of S, such that the data induced by T_{ab} on S is that of I and the data induced on some compact subjset of S' is that on C' in I'. That is, we consider the case of general relativity, but with no gravitational field.

First note that, were the energy conditions omitted above, we would have immediately that $I \rightarrow I'$ always. This follows from the fact that, locally, any conserved stress-energy in Minkowski space-time can be written as $T^{ab} = \nabla_m \nabla_n R^{ambn}$, where R^{ambn} is any tensor field having the

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algebraic symmetries of a Riemann tensor. But this potential can be adjusted arbitrarily from one Cauchy surface to the other.

Since there are no white holes in the absence of gravitational fields, one might have though that we would still have $I \rightarrow I'$ always even with the restriction to reasonable matter, in the sense of the energy conditions above. Unfortunately, this fails. The physical reason is that conservation of total energy-momentum now comes into play, since the energy condition requires that matter not travel faster than light, and so not come in from spatial infinity. This observation is made precise by the following.

Lemma: Let, in Minkowski space-time, T^{ab} be symmetric and conserved, satisfying the energy condition (3) everywhere, S and S' be Cauchy surfaces with S' to the future of S, and C' be any compact subset of S'. Then the total energy-momentum on $I^-(C') \cap S$ in S exceeds that on C' in S' by a future-directed timelike or null vector.

The proof is easy. Contract $\nabla_b T^{ab} = 0$ with any constant, future-directed timelike vector field and integrate, by parts, over $I^-(C') \cap I^+(S)$. *The boundary terms on* S and C' give the two total energy-momenta, while that on the null boundary between the Cauchy surfaces is non-negative, by (3). As an example, let I have $\mu = 0$ and $J^a = 0$. Then, by the Lemma, $I \rightarrow I'$ only for $I' = I$.

This lemma can also be used to illustrate why it is convenient to "build" only compact regions of the final configuration. Suppose, in the definition above, compactness of the region C' of S' were omitted. Then, for I any initial-data set with μ vanishing nowhere, and I' any set with μ' of compact support, we would have $I \not\rightarrow I'$. The energy condition imposes, in a sense, a remnant of an initial-value formulation.

It is easy to avoid these difficulties associated with conservation. For $I = (T, \mu, J^a)$ and $I' = (T', \mu', J^{a'})$ initial-data sets, we say that I has *sufficient energy-momentum* for I' if, given any compact subset C' of T', there is a compact subset C of T such that the total energy-momentum on C exceeds that on C' by a future-directed timelike vector. This condition, in short, guarantees that the lemma will represent no obstruction to building.

So, provided we demand that there be sufficient energy-momentum, is it then true that always $I \rightarrow I'$? The answer, as it turns out, is still no. Consider first initial data for a null fluid, i.e., $J^a = \mu v^a$, with $\mu \geqslant 0$ and v^a constant and unit. It follows from the lemma that the only conserved T_{ab} in Minkowski space-time satisfying the energy condition (3) and inducing on a flat slice this data is that corresponding to evolution of the data as a null fluid. That is, we recover, for this degenerate choice of data, a full initial-value formulation. Now consider data I consisting of two separated pieces of null fluid going in opposite directions, i.e., $J^a = \mu v^a$ in one region and $J^a = -\mu v^a$ in another, with these two regions separated by a 2-plane orthogonal to v^a. Again, the only evolution is that as a null fluid. But for this I the total energy-momentum is strictly timelike. Hence, there is sufficient energy-momentum for I' consisting, say, of data for a small, static, spherical fluid ball. Yet, while there is sufficient energy-momentum, we do not have $I \rightarrow I'$.

It seems likely that such examples—in which I consists of certain arrangements of regions of null fluid—are unstable, in the sense that certain strategically placed but arbitrarily small amounts of non-null matter will permit $I \rightarrow I'$ for reasonable I'. Further, it seems likely that these are the only remaining counterexamples. Thus, we may conjecture that, whenever I has sufficient energy-momentum for I', and I is "not regions of null fluid" in a suitable sense, then $I \rightarrow I'$. One precise version of "not regions of null fluid"—perhaps somewhat stronger than necessary—is to demand that (2) be a strict inequality wherever $\mu \neq 0$. The physical idea of the proof would be to use some of the matter of the initial-data set I to construct rubber bands to collect the matter into a confined region, forming eventually a static spherical fluid ball. Then, reversing this procedure, one would reconstruct from the fluid ball a given compact region of the initial-data set I'. Unfortunately, translating this idea into a full proof seems to be difficult. In any case, it appears to be the case that, subject to these caveats, anything can be built from anything in the theory of test stress-energies.

The discussion above illustrates the impact of sources on the notion of building. As a second example, to illustrate the impact of radiation, consider electromagnetism. Let an initial-data set I consist of vector fields E^a and B^a, the latter divergence-free, in Euclidean 3-space T. Write $I \rightarrow I'$ if, given any compact region C' of T', there exists in Minkowski space-time a solution of Maxwell's equations (possibly with nonzero charge-current), together with flat parallel spacelike Cauchy surfaces, S' to the future of S, such that the data induced on S by the Maxwell field is that of I and the data induced on some compact region of S' is that of I' on C'. Stated in this way, it follows immediately that any initial-data set can be built from any other in electromagnetism. Indeed, the most general Maxwell field is the curl of an arbitrary vector potential. One merely adjusts that potential smoothly from the value determined by the data on S to that on S'. Thus, there are no additional conditions over and above the field equations to be imposed in electromagnetism. There are no "Maxwell white holes" to be argued against on other grounds.

Of course, the key difference between general relativity and electromagnetism is that there is nothing in the latter analogous to the energy condition in the former. One can force a closer analogy—at sacrifice of physical content—by modifying the electromagnetic case as follows. Demand, of the charge-current vector for the Maxwell field in Minkowski space-time, that it be future-directed timelike or null; and correspondingly demand of each initial-data set that $\rho = D_a E^a$ be non-negative. That is, one deals with charges having only one sign. What now happens is similar to that of the case of test stress-energy. The lemma is replaced by an analogous statement, with analogous proof, but with "total charge" replacing "total energy-momentum". We say that $I = (T, E^a, B^a)$ has *sufficient charge* for $I' = (T', E^{a'}, B^{a'})$ if, given any compact subset C' of T' there exists a compact subset C of T such that the total charge on C exceeds that on C'. There appears to be nothing in the electromagnetic case analogous to the "regions of null fluid" in the case of test stress-energies.

So, in view of the remarks above, one might suspect that, provided I has sufficient charge for I', we shall have $I \to I'$. But this, too, fails. For example, let I' be the initial-data set with $E'^a = B'^a = 0$. Let I have $E^a = E_1^a + E_2^a$ and $B^a = B_1^a + B_2^a$. Let E_1^a be the Coulomb electric field of a small spherical charge distribution, of total charge q, centered at the origin, and $B_1^a = 0$. Let E_2^a, B_2^a represent two plane waves, on either side of the origin, directed toward the origin. That is, in Euclidean coordinates, let $B_2^a = f(x^2) z^a$, where f is a non-negative rapidly increasing function of its argument, vanishing at zero, and $E_2^a = f(x^2)\hat{y}^a$ or $-f(x^2)\hat{y}^a$ for x negative or positive, respectively. Now, I clearly has sufficient charge for I' and yet, we claim, I' cannot be built from I. A sketch of the proof follows. Suppose, for contradiction, that $I \to I'$. Choose, for the compact region C' of T' on which the data of I' is to be reproduced, a ball of large radius r centered at the origin. Let E^a and B^a be the resulting electric and magnetic fields in space-time (so, e.g., these must vanish in C'), and $t \gg r$, the time-separation between the two slices. Next note that, for $\tilde{E}^a$, $\tilde{B}^a$ any solution of Maxwell's equations with vanishing sources, we have

$$\frac{d}{dt}(E^a\tilde{E}_a + B^a\tilde{B}_a) + D_a(\epsilon^{amn}(E_m\tilde{B}_n + \tilde{E}_m B_n)) = J^a\tilde{E}_a, \tag{4}$$

where J^a is the current density of E^a, B^a. Now choose $\tilde{E}^a$, $\tilde{B}^a$ such that $\tilde{E}^a$ vanishes on T', $\tilde{B}^a$ vanishes outside of C' on T', and $\tilde{B}^a$ is a positive multiple of z^a in C'. Integrating (4) over the region of space-time between the slices, we obtain

$$\int_T (E^a\tilde{E}_a + B^a\tilde{B}_a) = \int_{[T,T']} J^a\tilde{E}_a. \tag{5}$$

But, by our choice of fields, the left side is bounded below by essentially $f(t^2)$ while, since the charge-current must be future-directed timelike or null, the right side is bounded above by essentially tq. This contradicts our choice of f.

The physical idea behind this example is clear. One wishes to expunge the fields from the region C' of size r at some time t. This is to be done by manipulating a total charge q. But, with no efforts at manipulation, the field strengths will grow very quickly in time, because of the imploding plane-waves with strength determined by f. With only finite charge available, no manipulations can succeed at any future time over the plane waves.

The key to this example is the presence, on I, of incoming radiation of increasing intensity. This suggests that we shall always have $I \to I'$, provided I has sufficient charge for I', *and* each satisfies suitable boundary conditions. This is true. Given I, I', and the compact region C' of T', assemble a sufficient amount of charge of I into a large spherical ball of uniform density. Next, hold this charge in this configuration, and the remaining charges of I fixed, for a sufficiently large time that the radiation incident on the ball (from the initial data on I in the asymptotic region) becomes small. Then, distribute a small amount of charge about the surface of the ball to cancel out any future incoming radiation. The result is that, after some finite time, the field inside the ball will be maintained as the static electric field of the uniform charge distribution. Finally, just reverse this process to reconstruct the data to be produced on the region C' of T'.

3. DISCUSSIONS

We now turn to the central issue—that of providing a suitable definition of "buildable objects" in general relativity. The definition of the Introduction should serve this purpose, provided that two additional conditions, as suggested by the examples of the previous section, are appended.

First, the example of electromagnetism suggests that there should be imposed boundary conditions on the initial-data sets considered. Otherwise, it seems likely, the definition would not capture the intended meaning, for a rather benign final configuration could not be built from an initial configuration with strong incoming radiation. Fortunately, the formulation of such a condition should pose no difficulties, for there are available several definitions of asymptotic flatness at spatial infinity.[5]

Second, the example of test stress-energies in Minkowski space-time suggests that there should be imposed on the initial-data sets a condition reflecting "sufficient energy-momentum". That some such condition is appropriate even in the presence of curvature is illustrated by the following observation. Let I be any initial-data set with vanishing sources, and I' any set with sources somewhere nonvanishing. Then, as an immediate consequence of a theorem of Hawking,[6] I' cannot be built from I. The problem, however, is that it is by no means clear how a suitable condition is to be formulated: The "total energy-momentum of the matter," which plays the central role in the case of a test stress-energy, is normally regarded as undefined in the presence of gravitation. One possible line of attack would be to make use of Witten's expression[7] for the total energy-momentum of an isolated system, an expression which separates naturally into field and matter contributions.

As an illustration of this issue, we given an example of a simple, natural question one would wish to be able to answer. Let I be initial data for a static spherical fluid ball of matter, of total mass M, and I' data for a similar ball of mass M', with $M' > M$. Can I' be built from I? That is, can a large star be built from a small star? Intuitively, one would expect not, and indeed one can prove not with the additional condition that the intervening space-time be spherically symmetric. But the full question apparently remains open.

Finally, we remark that there is in fact a result to the effect that "white holes cannot be built from ordinary matter". Let I be initial data for a static, spherical fluid ball ("ordinary matter"), and I' data with a past trapped surface ("white hole"). Then I' cannot be built from I, for if so the corresponding solution of Einstein's equation would violate a singularity theorem.[8]

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Relationship between the inverse scattering techniques of Belinskii–Zakharov and Hauser–Ernst in general relativity [a]

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We make a quantitative comparison between the *pure-nonsoliton* part of the inverse scattering method of Belinskii and Zakharov (BZ) and the homogeneous Hilbert problem of Hauser and Ernst (HE), these being two independent representations of an infinite-dimensional subgroup $\mathscr{K}$ of the Geroch group **K** of invariance transformations for spacetimes with two commuting Killing vectors. An explicit formula for the BZ representing matrix function $G_0(\lambda)$ in terms of the HE representing matrix function $u(t)$ is derived. It is shown how certain solution generating techniques (e.g., Harrison's Bäcklund transformation, HKX transformation, generation of Weyl solution from flat space, generation of n-Kerr–NUT solution from n-Schwarzschild) can be derived directly from the BZ formalism, including the soliton part in some cases, thereby bringing our understanding of the BZ formalism up to the level of the more fully developed HE formalism. A technical point which needed to be resolved along the way was how to analytically continue the complex matrix potential $F(t)$ across a quadratic branch cut and onto the second Riemann sheet. Finally, we consider how the subgroup $\mathscr{K} \subset \mathbf{K}$ represented by the BZ and HE formalisms can be enlarged either by simple limiting transitions or by relaxing boundary conditions.

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1. INTRODUCTION AND PRELIMINARY

The "inverse scattering" technique is an attractive and powerful formalism for solving certain systems of nonlinear partial differential equations of mathematical physics. The essential feature of the method is to write down an overdetermined system of linear eigenvalue equations (a so-called L–A pair) whose integrability conditions are the given nonlinear system. Then methods of functional analysis can be applied to generate new solutions of the linear system from old, and hence new solutions of the original system from old. Most if not all of the partial differential equations which are known to yield to the inverse scattering method also exhibit other remarkable phenomena such as an infinity of conservation laws, Bäcklund transformations, Bianchi diagrams, and nonlinear superposition principles.[1]

In the case of Einstein's gravitational field equations with two commuting Killing vectors, there are two rival inverse scattering methods found independently by Belinskii and Zakharov[2] (BZ) and Hauser and Ernst[3–5] (HE). The latter provide an explicit representation of the infinite-dimensional Geroch group[6] **K** of invariance transformations (strictly speaking, a large subgroup $\mathscr{K}_L$ of $\mathbf{K}$[5]) and was derived initially from the earlier representation of the associated Lie algebra given by Kinnersley and Chitre[7–10] (KC). The HE formalism has been developed and applied in a series of papers,[3–5,11] some of the highlights of which are the following: reduction of certain ingenious solution-generation techniques of Kinnersley and coworkers (e.g., flat space→Weyl,[9] Schwarzschild→Kerr,[10] HKX transformation[12]) to relatively simple problems in complex-variable theory[3,4]; a proof of Geroch's conjecture[6] that the **K** group is (multiply) transitive on the space of solutions in a certain well-defined sense[5]; and recognition that Harrison's Bäcklund transformation[13,14] is contained in the **K** group.[11] Belinskii and Zakharov[2] separate invariance transformations into "soliton" and "nonsoliton" parts, these ideas being taken from the theory of certain nonlinear wave equations (or their elliptic counterparts) in quantum physics.[1] Subsequent papers[15] have concentrated almost exclusively on the *pure-soliton* BZ transformations which are permutable Bäcklund transformations and have been shown to be closely related to the Harrison and HKX transformations.[16]

It is apparent at a glance that the HE formalism and the *pure-nonsoliton* part of the BZ formalism are qualitatively similar: both reduce the nonlinear field equations to an homogeneous Hilbert problem (HHP) or regular Riemann problem in complex functional analysis. However, the problem of providing quantitative mathematical formulas connecting the two formalisms is far from straightforward even though the exact relation between the respective eigenfunctions $F(t)$ and $\psi(\lambda)$ is known[16] (see Appendix B). What is needed is an explicit formula for the BZ representing matrix function $G_0(\lambda)$ ("scattering data") in terms of the HE representing matrix function $u(t)$. The result [Eq. (2.35) below] shows how a particular transformation in one formalism can be written in the other.

In Sec. 3, we show how to solve the BZ homogeneous Hilbert problem for four special classes of $G_0(\lambda)$ matrices. They are (A) Harrison's Bäcklund transformation,[13,14] (B) the null generalized HKX transformation,[12,16] (C) generation of the general Weyl or Einstein–Rosen solution from flat space,[9] and (D) **B**-group[10] generation of the nonlinear superposition of n Kerr–NUT particles from n Schwarzschild particles. The first three examples can be directly com-

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pared with the corresponding calculations in the HE formalism. The fourth case, however, is quite different and belongs in the pure-soliton framework.

Before the explicit relation (2.35) connecting $G_0(\lambda)$ to $u(t)$ can be constructed, it will be necessary to make precise the assumptions about gauge, analyticity properties, and boundary conditions used in the BZ formalism. In particular, the boundary condition, $G_0(\infty) = I$ (unit 2×2 matrix) in Ref. 2 will be dropped as it is unnecessarily restrictive, and the requirement of symmetry of $G_0(\lambda)$ will be replaced by a more complicated symmetry condition in order to achieve internal consistency. The chosen boundary conditions, etc., were motivated by the corresponding conditions chosen by Hauser and Ernst. Hauser and Ernst have also studied the analyticity properties of the $F(t)$ potential in the complex t plane.[4,5] In order to understand the analyticity properties of the corresponding BZ eigenfunction $\psi(\lambda)$ in the complex λ plane, we need the exact form of the analytic continuation of $F(t)$ across a quadratic branch cut in the t plane and onto the second Riemann sheet. This problem is solved in Appendix A using some powerful ideas in Ref. 5.

With the boundary conditions and other assumptions in Sec. 2, the solutions of the HHP's for given $u(t)$ or $G_0(\lambda)$ are guaranteed to be unique. However, some of these conditions can be relaxed with the result that the solutions are no longer unique, but may depend on some arbitrary "constants" which are actually arbitrary functions of the spacetime coordinates. One must then substitute the class of solutions admitted by the HHP's directly into Einstein's equations and/or the equivalent eigenvalue equations in order to see which are genuine gravitational solutions (the final solutions may be unique or contain some integration constants). The mixed soliton and nonsoliton transformations of Belinskii and Zakharov[2] are an example of this phenomenon where the functions $\chi_1(\lambda)$ and $\chi_2(\lambda)$ or their inverses are allowed to have poles in the regions of the λ plane where they would be required to be analytic in the case of a pure-nonsoliton transformation. It is not clear, when the rules have been so changed, whether the pure-soliton and mixed transformations are in **K** itself or some larger group.[17] In fact, the $2n$-soliton transformation is necessarily in **K** because it is identical (up to some gauge and trivial transformations) to the $2n$-fold Harrison transformation[16] which is known to be in **K**.[11] In Ref. 16, we also proved that the $(2n-1)$-soliton transformation is the product of $2n-1$ Harrison transformations and the Kramer–Neugebauer involution[18] in any order. In Sec. 4, we discuss the possibility of including the Kramer–Neugebauer involution in a suitable analytic continuation of the subgroup $\mathscr{K}_L \subset \mathbf{K}$ represented by the HE formalism.

In Sec. 4, we also discuss more straightforward analytic continuations of $\mathscr{K}_L$ which can be represented in the HE formalism by relaxing boundary conditions at $t=\infty$. A simple example is the $s=\infty$ limit of the null (and nonnull) HKX transformation which was calculated in Ref. 16 by exponentiating the appropriate limiting infinitesimal transformation. In the HE formalism, the null HKX transformation with finite s is represented by a $u(t)$ matrix with a simple pole at $t=s$ *inside* the closed contour L. The limiting HKX transformation can be derived from an HHP with $u(t)=I$ and $X_-(t) = O(t)$ as $t\to\infty$, and an additional parameter can be incorporated by also allowing $u(t) = O(t)$ as $t\to\infty$. As in the case of the BZ soliton transformations, the solution of this modified HHP involves an arbitrary matrix function of the space-time coordinates which must be determined by substitution into Einstein's equations. By taking limits of more complicated transformations as singularities of $u(t)$ go to infinity, it is clear that $u(t)$ and $X_-(t)$ can be allowed to have virtually any type of singularity at $t=\infty$, including branch points and nonisolated essential singularities. The special boundary conditions at $t=\infty$ on $u(t)$ and $X_-(t)$ chosen by Hauser and Ernst are thus seen to be not necessary for the preservation of Einstein's equations but have the convenient property of guaranteeing uniqueness of the solution of the HHP for given $u(t)$ and input $F(t)$.

The gravitational field equations in the presence of two commuting Killing vectors, which are reducible to the Ernst equation[19] for a complex potential $\mathscr{E}$, are applicable to many problems both within and outside the general theory of relativity. For example, they apply to stationary axisymmetric vacuum fields,[20] cylindrical wave fields,[21] the interaction region of colliding plane waves,[22] electrostatic and magnetostatic Einstein–Maxwell fields,[23] classical nonabelian gauge theories,[24] self-dual Yang–Mills fields,[25] and are closely related to the principal chiral fields.[26] The largest body of literature applies to the case of stationary axisymmetric vacuum gravitational fields, but most of the results in one theory can be shared with the others.[27] In this paper, we wish to treat the stationary axisymmetric and cylindical wave cases together, keeping in mind that there is a simple complex coordinate transformation that maps one case onto the other. Also, many of the references already cited (e.g., some of Refs. 3, 4, 7–9, 11, 15) consider extensions of the theory of the **K** group or solitonic methods to stationary axisymmetric electrovac Einstein–Maxwell fields, but only the vacuum case will be treated in the present paper.

The canonical form of the metric of stationary axisymmetric space-time is[7,20]

$$ds^2 = f_{AB}dx^A dx^B - e^{2\Gamma}(d\rho^2 + dz^2), \tag{1.1}$$

$A,B = 1,2, f_{11}f_{22} - (f_{12})^2 = -\rho^2$, where x^1, x^2, ρ, and z are time, azimuthal, radial, and axial coordinates, respectively, and f_{AB} and Γ are functions of ρ and z only. A change of variable,

$$\alpha = i\rho, \quad \beta = z, \tag{1.2}$$

(and change of sign of ds^2 to preserve signature -2) puts the metric in the form appropriate to cylindrically symmetric gravitational waves:

$$ds^2 = -f_{AB}dx^A dx^B + e^{2\Gamma}(-d\alpha^2 + d\beta^2). \tag{1.3}$$

Here, $f_{11}f_{22} - (f_{12})^2 = \alpha^2$, f_{AB} and Γ are functions of α and β only, and x^1, x^2, α, and β are axial, azimuthal, radial, and time coordinates, respectively. The coordinates α and β are to be identified with the fields $\alpha(\zeta,\eta)$ and $\beta(\zeta,\eta)$ of Ref. 2. When the BZ formalism is under consideration, we shall use the metric form (1.3) exclusively (Sec. 3D excepted), whereas in the HE formalism, we shall use (1.1) and (1.3) interchangeably.[27] The function Γ, which can be calculated from f_{AB} by quadrature, will play no further role in this paper.

When a particular solution of the elliptic (stationary case) or hyperbolic (wave case) field equations governing f_{AB} is given, a number of other important auxiliary potentials can be calculated. We refer the reader to the literature, especially Refs. 3–5, 7–10, and 16, for the field equations and defining relations for potentials and Refs. 2, 13–16, and 28 for pseudopotentials and eigenfunctions. We use the matrix notation,

$$\mathbf{g} = (f_{AB}) = \begin{pmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{pmatrix} = \begin{pmatrix} f & -f\omega \\ -f\omega & f\omega^2 - \rho^2 f^{-1} \end{pmatrix}, \tag{1.4}$$

and so $\mathbf{g}$ is symmetric and

$$\det \mathbf{g} = -\rho^2 \quad \text{or} \quad \alpha^2. \tag{1.5}$$

The SL(2)-tensor notation used extensively in Refs. 7–10 and 16 will not be used here except for brief appearances in Secs. 3B and 4. From the real matrix potential $\mathbf{g}$, one can construct a complex matrix potential,[7]

$$H = (H_{AB}) = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}, \tag{1.6}$$

[see Eq. (A2)] for which

$$\mathbf{g} = \operatorname{Re} H \quad \text{or} \quad f_{AB} = \operatorname{Re} H_{AB}, \tag{1.7}$$

and $H_{12} - H_{21} = 2iz$ or $2i\beta$. The 11 component of H is the complex Ernst potential,[19]

$$\mathscr{E} = H_{11} = f + i\psi. \tag{1.8}$$

The inverse scattering technique is applicable to this problem because it is possible to construct a complex matrix potential ("eigenfunction") $F(t)$[3–5,9–12,16,29] which is a nontrivial function of *three* variables, (ρ,z,t) or (α,β,t), by solving a simple linear partial differential equation, Eq. (A1) (or nonlinear characteristic equation[10] or Riccati equation[16]). This was originally introduced in Ref. 9 as a generating function of potentials,

$$F(t) = i\boldsymbol{\epsilon} + tH + t^2 H^{(2)} + t^3 H^{(3)} + \cdots \tag{1.9}$$

[cf. Eqs. (A6a,b)], where

$$\boldsymbol{\epsilon} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{1.10}$$

Hauser and Ernst used $F(t)$ as their basic field variable and determined some of its analyticity properties in the complex t plane (t may be called a "spectral parameter.") There is the important result:

Theorem (Hauser and Ernst[5]): In a (ρ,z) domain containing the origin (0,0) for which $\mathscr{E}$ is an analytic function of (ρ,z) and $f \neq 0$, there is a unique gauge for $F(t)$ such that $F(t)$ is analytic in the whole complex t plane and

$$F(t) \begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix} \text{ is analytic at } t = \infty, \tag{1.11}$$

except for two quadratic branch points of index $-\frac{1}{2}$, joined by a cut, at the zeros of

$$S(t) = [(1 - 2tz)^2 + 4t^2\rho^2]^{1/2}, \quad S(0) = 1. \tag{1.12}$$

We shall call this gauge "special HE gauge" as in Ref. 11. A change of gauge [see Eqs. (A5) and (A8)] introduces (ρ,z)-independent singularities in the finite t plane and/or at $t = \infty$.[30] If $\mathscr{E}$ is analytic and $f \neq 0$ at a point $(0,z_0)$ of the z axis, but not at (0,0), we assume that the regular point has been brought to the origin by a translation, $z \to z - z_0$. If $\mathscr{E}$ is singular and/or $f = 0$ along the whole z axis, then the minimally singular form of $F(t)$ may be quite different [see Eq. (4.27) below and Ref. 4]. Analytic continuation of $F(t)$ in special HE gauge across the branch cut and onto the second Riemann sheet will reveal (ρ,z)-independent singularities at $t = 0$ and in places that depend on the functional form of $\mathscr{E}(0,z)$. The exact functional relation between the two values of $F(t)$ on the two Riemann sheets [we write $\tilde{F}(t)$ for the second sheet] is calculated in Appendix A.

Belinskii and Zakharov use a different matrix potential, $\psi(\lambda) = \psi(\alpha,\beta,\lambda)$, and different spectral parameter λ whose relations to $F(t)$ and t, respectively, are discussed in Ref. 16 and Appendix B here. Note that the complex λ plane maps onto the double-sheeted Riemann t surface which is the domain of the function,

$$S(t) = [(1 - 2t\beta)^2 - 4t^2\alpha^2]^{1/2}, \quad S(0) = 1. \tag{1.12$'$}$$

We restrict attention to (α,β) domains for which $|\beta| > \alpha > 0$ so that the image of the circle $|\lambda| = \alpha$ is the finite line segment along the real axis of the t plane joining the zeros of $S(t)$ traced in both directions and not passing through $t = 0$. The λ-values, λ and α^2/λ, map to the same t-values, but on different Riemann sheets. Appendix B gives the exact functional relation between $\psi(\lambda)$ and $\psi(\alpha^2/\lambda)$.

Finally, we wish to discuss briefly the homogeneous Hilbert problem (HHP) posed by Hauser and Ernst to provide simultaneously an explicit representation of a large subgroup ($\mathscr{K}_L$ of Ref. 5) of the Geroch group $\mathbf{K}$ and a practical method of generating new solutions from old. The reader is referred to Refs. 3–5 for a more detailed treatment, and Ref. 11 for notations and conventions.[29]

The transformation group $\mathscr{K}_L \subset \mathbf{K}$ is isomorphic to the Lie group of 2×2 matrix functions $u(t)$ of a complex variable t, subject to the conditions:

$$\det u(t) = 1; \tag{1.13a}$$

$$u(t) \quad \text{is real for real } t; \tag{1.13b}$$

$$u(t) \quad \text{is analytic in a neighborhood of } t = \infty; \tag{1.13c}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & t^{-1} \end{pmatrix} u(t) \begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix} \quad \text{is analytic at } t = \infty. \tag{1.13d}$$

The group product is the usual matrix product. Next, draw a simple closed contour L in the complex t plane enclosing all the singularities of $u(t)$ and symmetric about the real axis. The interior of L is denoted L_+ and the exterior L_-. Then choose a particular gravitational solution f_{AB} or equivalent solution $\mathscr{E}$ of the Ernst equation[19] and calculate the $F(t)$ potential *in special HE gauge*. Restrict the (ρ,z) domain to a region sufficiently close to (0,0) so that the two quadratic branch points of $F(t)$ and the cut joining them lie wholly in L_-. So $F(t)$ is analytic in $L + L_+$ and $u(t)$ is analytic in $L + L_-$.

A new solution $\mathscr{E}'$, together with associated potential $F'(t)$ in special HE gauge, which is the transform of $\mathscr{E}$ under the element of $\mathscr{K}_L$ represented by $u(t)$ can be calculated by solving the following homogeneous Hilbert problem: determine a matrix function $X_-(t)$ analytic in $L + L_-$ and a matrix function $X_+(t)$ or, equivalently, $F'(t) = X_+(t)F(t)$, analytic in $L + L_+$ such that

$$X_-(t) = X_+(t)F(t)u(t)F(t)^{-1}$$
$$= F'(t)u(t)F(t)^{-1}. \tag{1.14}$$

The boundary conditions are

$$X_+(0) = I, \quad F'(0) = i\epsilon, \tag{1.15a}$$

$$X_-(t) \quad \text{is analytic at} \quad t = \infty. \tag{1.15b}$$

The solution exists and is unique.[5]

A consequence of the use of special HE gauge is that the above construction of the transformation group $\mathscr{K}_L$ is independent of the contour L: henceforth we drop the subscript L on $\mathscr{K}_L$. In fact, it is sufficient to specify that $F'(t)$ or $X_+(t)$ be analytic in the whole t plane except for two branch points joined by a cut at the zeros of $S(t)$ and satisfy conditions (1.15a) and (1.11) and that $X_-(t)$ be analytic at the two branch points of $S(t)$ and at $t = \infty$. This construction does not admit gauge transformations in **K** of the form (A5) (except for $\mathscr{E} \to \mathscr{E} + i\psi_0$, ψ_0 real constant). Also, as already mentioned, a larger subgroup of **K** can be represented by relaxing the boundary conditions at $t = \infty$ (see Sec. 4).

2. THE HOMOGENEOUS HILBERT PROBLEM OF BELINSKII AND ZAKHAROV AND THE FORMULA FOR $G_0(\lambda)$ IN TERMS OF $u(t)$

The pure-nonsoliton part of the inverse scattering technique of Belinskii and Zakharov[2] is a representation of a subgroup of **K** (at least as large as $\mathscr{K}$) in the form of an homogeneous Hilbert problem qualitatively similar to that of Hauser and Ernst.[4,5] In this section, we determine the exact quantitative relationship between the BZ and HE formalisms, but first we must set up the correct boundary conditions for the BZ HHP and establish the analyticity properties of the BZ eigenfunction $\psi(\lambda)$. The spectral parameter λ is related to t by the quadratic transformation discussed in the first paragraph of Appendix B.

The respresenting matrix in the BZ formalism is a nondegenerate (i.e., possessing an inverse) 2×2 matrix function $G_0(\lambda)$, which is a function of α, β, and λ such that, when written as a function of α, β, and t using (B3a,b) *is a function of t only*,[31] and is real for real t. We shall *not* use the BZ conditions,[2]

$$G_0(\lambda) \quad \text{is symmetric}, \quad G_0(\infty) = I, \tag{2.1a,b}$$

as the former will be incompatible with our choice of gauge and the latter is unnecessarily restrictive: instead, we shall derive alternative conditions from first principles. We shall in future write $G_0(t)$ for this representing matrix, with the understanding that t is given by the right-hand side of Eq. (B1). $G_0(t)$ may have (α,β)-independent singularities anywhere in the complex t plane, but not branch points at the zeros of $S(t)$. Choose an (α,β) domain with $|\beta| > \alpha$ such that $G_0(t)$ is analytic on the circle $|\lambda| = \alpha$, to be denoted Γ.[32] Let the interior of Γ be denoted Γ_2, exterior Γ_1.

The BZ eigenfunction $\psi(\lambda)$, a function of α, β, and λ or t, is related to $F(t)$ by[16]

$$\psi(\lambda) = t^{-1}S(t)\,\mathrm{Re}\,F(t), \tag{2.2}$$

for $|\lambda| < \alpha$, and its analytic continuation to $|\lambda| > \alpha$ is determined in Appendix B. In particular,

$$\psi(0) = \mathbf{g} = \mathrm{Re}\,H. \tag{2.3}$$

We impose special HE gauge on $F(t)$. As a result, $\psi(\lambda)$ is analytic everywhere in Γ_2 and on Γ. Furthermore, condition (1.11) implies

$$\psi(\lambda)\begin{pmatrix}1 & 0\\ 0 & (\lambda-\lambda_2)^{-1}\end{pmatrix} \quad \text{is analytic at } \lambda = \lambda_2, \tag{2.4}$$

where λ_2 is the zero of $\lambda^2 + 2\beta\lambda + \alpha^2$ in Γ_2, and λ_1 is the other zero in Γ_1. If $\mathscr{E}$ is sufficiently well behaved at $(\alpha,\beta) = (0,0) = (\rho,z)$, then a similar condition holds at $\lambda = \lambda_1$. Condition (2.4) will later necessitate a boundary condition on $G_0(t)$ at $t = \infty$ (i.e., at $\lambda = \lambda_{1,2}$):

$$\begin{pmatrix}1 & 0\\ 0 & t^{-1}\end{pmatrix} G_0(t) \begin{pmatrix}1 & 0\\ 0 & t\end{pmatrix} \quad \text{is analytic at } t = \infty. \tag{2.5}$$

The BZ HHP is to find $\chi_1(\lambda)$ analytic and nondegenerate in $\Gamma + \Gamma_1$ and at $\lambda = \infty$ and $\chi_2(\lambda)$ analytic and nondegenerate in $\Gamma + \Gamma_2$, such that, on Γ,

$$\chi_1(\lambda) = \chi_2(\lambda)G(\lambda), \tag{2.6a}$$

where

$$G(\lambda) = \psi(\lambda)G_0(t)\psi(\lambda)^{-1}. \tag{2.6b}$$

We use a prime to denote transformed variables. The new metric $\mathbf{g}'$ and eigenfunction $\psi'(\lambda)$ in special HE gauge are given by

$$\psi'(\lambda) = \chi_2(\lambda)\psi(\lambda), \quad \mathbf{g}' = \psi'(0) = \chi_2(0)\mathbf{g}. \tag{2.7a,b}$$

In addition to the HHP, Belinskii and Zakharov also impose an auxiliary functional relation,

$$\mathbf{g}' = \chi_1(\alpha^2/\lambda)\mathbf{g}\chi_2(\lambda)^T, \tag{2.8}$$

^{T} denoting matrix transpose, which is compatible with the HHP and our choice of gauge. [It will be seen to be related to Eq. (75) of Ref. 4.] The transpose of Eq. (2.8) is

$$\mathbf{g}' = \chi_2(\lambda)\mathbf{g}\chi_1(\alpha^2/\lambda)^T. \tag{2.9}$$

Now put $\lambda = 0$ in Eq. (2.9) and compare with Eq. (2.7b): we find

$$\chi_1(\infty) = I. \tag{2.10}$$

This the boundary condition at $\lambda = \infty$ that we shall use. It is intended to replace the BZ conditions (2.1b) and $\chi_2(\infty) = I$, which are more restrictive. In fact, we do not require $G_0(t)$ or $\chi_2(\lambda)$ to be analytic at $\lambda = \infty$, and so the HHP is not necessarily "canonical."[26]

The *mixed soliton–nonsoliton* transformations[2] are solutions of a generalization of the above HHP in which $\chi_2(\lambda)$ is allowed to have poles at specified points, $\lambda = \mu(s_1),\ldots,\mu(s_n)$, in Γ_2 and so, from Eq. (2.8), $\chi_1(\lambda)$ is degenerate at $\lambda = \nu(s_1),\ldots,\nu(s_n)$ in Γ_1 [see Eqs. (B3a,b)]. The solution of this generalized HHP is not unique and it is necessary to resort to the differential equation[2] for $\psi'(\lambda)$ to identify the residues of $\chi_2(\lambda)$ at the poles in Γ_2. The *pure-soliton* transformations, as yet the only case discussed in any detail in the literature,[2,15,16] are the special cases of the mixed transformations for which

$$G_0(t) = I, \quad \chi_1(\lambda) = \chi_2(\lambda). \tag{2.11}$$

Before discussing the determinant of $G_0(t)$, we must recall from Ref. 2 that the BZ formalism does not guarantee the relations

$$\det \mathbf{g}' = \alpha^2, \quad \det \boldsymbol{\psi}'(\lambda) = \lambda^2 + 2\beta\lambda + \alpha^2 = \lambda/t \tag{2.12a,b}$$

for the transformed solution. In fact, it is well known that Eqs. (2.12a,b) do not hold in the pure-soliton case and so could not hold, in general, in the mixed soliton–nonsoliton case. In any case, however, a "physical" metric and eigenfunction satisfying *all* of the field equations and eigenvalue equations can be constructed from the rescalings[2,16]:

$$\mathbf{g}'_{\rm ph} = \alpha(\det \mathbf{g}')^{-1/2}\mathbf{g}', \tag{2.13a}$$

$$\boldsymbol{\psi}'_{\rm ph} = (\lambda/t)^{1/2}(\det \boldsymbol{\psi}')^{-1/2}\boldsymbol{\psi}' = (\det \boldsymbol{\chi}_2)^{-1/2}\boldsymbol{\chi}_2\boldsymbol{\psi}. \tag{2.13b}$$

It is easy to see that Eqs. (2.12a,b) hold in the pure-nonsoliton case provided

$$\det G_0(t) = 1. \tag{2.14}$$

We shall show that condition (2.14) can be imposed on $G_0(t)$ without loss of generality in all cases. The nonmatrix HHP,

$$\theta_1(\lambda) = \theta_2(\lambda) \det G_0(t), \quad \theta_1(\infty) = 1, \tag{2.15}$$

$\theta_{1,2}$ analytic and nonvanishing in $\Gamma_{1,2}$, respectively, has the unique solution,

$$\theta_{1,2}(\lambda) = \exp\left\{ -\frac{1}{2\pi i}\int_\Gamma \frac{D(\lambda')}{\lambda' - \lambda}\, d\lambda'\right\}, \quad \lambda\in\Gamma_{1,2}, \tag{2.16a}$$

where

$$D(\lambda) = \ln \det G_0(t) = D(\alpha^2/\lambda) \tag{2.16b}$$

[note that no branch cuts of $D(\lambda)$ intersect the circle Γ]. The change of variable, $\lambda' \rightarrow \alpha^2/\lambda''$, in Eqs. (2.16a) yields the functional relation,

$$\theta_1(\alpha^2/\lambda) = \theta_2(0)/\theta_2(\lambda). \tag{2.17}$$

Define

$$\bar{G}_0(t) = [\det G_0(t)]^{-1/2}G_0(t), \quad \bar{G}(\lambda) = \boldsymbol{\psi}(\lambda)\bar{G}_0(t)\boldsymbol{\psi}(\lambda)^{-1}, \tag{2.18a,b}$$

$$\bar{\boldsymbol{\chi}}_1(\lambda) = \theta_1^{-1/2}(\lambda)\boldsymbol{\chi}_1(\lambda), \quad \bar{\boldsymbol{\chi}}_2(\lambda) = \theta_2^{-1/2}(\lambda)\boldsymbol{\chi}_2(\lambda), \tag{2.18c,d}$$

and observe that $\det \bar{G}_0(t) = 1 = \det \bar{G}(\lambda)$. Then the HHP for the pure-nonsoliton or mixed cases can be rewritten in terms of barred quantities:

$$\bar{\boldsymbol{\chi}}_1(\lambda) = \bar{\boldsymbol{\chi}}_2(\lambda)\bar{G}(\lambda), \tag{2.19a}$$

$$\bar{\boldsymbol{\psi}}'(\lambda) = \bar{\boldsymbol{\chi}}_2(\lambda)\boldsymbol{\psi}(\lambda) = \theta_2^{-1/2}(\lambda)\boldsymbol{\psi}'(\lambda), \tag{2.19b}$$

$$\bar{\mathbf{g}}' = \bar{\boldsymbol{\chi}}_1(\alpha^2/\lambda)\mathbf{g}\bar{\boldsymbol{\chi}}_2(\lambda)^T = \theta_2^{-1/2}(0)\mathbf{g}'. \tag{2.19c}$$

In the pure-nonsoliton case, we must identify

$$\theta_{1,2}(\lambda) = \det \boldsymbol{\chi}_{1,2}(\lambda), \tag{2.20}$$

and so

$$\det \bar{\boldsymbol{\chi}}_{1,2}(\lambda) = 1, \quad \bar{\mathbf{g}}' = \mathbf{g}'_{\rm ph}, \quad \bar{\boldsymbol{\psi}}'(\lambda) = \boldsymbol{\psi}'_{\rm ph}(\lambda). \tag{2.21a,b,c}$$

In the mixed or pure-soliton cases, we must still use Eqs. (2.13a,b) with barred quantities on the right-hand sides. In these cases, Eqs. (2.19a,c) imply

$$\Delta \equiv \det \bar{\boldsymbol{\chi}}_{1,2}(\lambda) = \frac{[\lambda - \nu(s_1)][\lambda - \nu(s_2)]\ldots[\lambda - \nu(s_n)]}{[\lambda - \mu(s_1)][\lambda - \mu(s_2)]\ldots[\lambda - \mu(s_n)]}, \tag{2.22}$$

in agreement with Eq. (5.16) of Ref. 16. In future, we accept condition (2.14) and drop the bars.

We now turn to the determination of the correct symmetry condition on the representing matrix $G_0(t)$. This will be deduced from the HHP (2.6a,b), the auxiliary relation (2.8), and the following functional relations which are proved in Appendices A and B:

$$\tilde{F}(t) = iF(t)h(t), \tag{2.23}$$

$$\boldsymbol{\psi}(\alpha^2/\lambda) = \lambda^{-1}\mathbf{g}\boldsymbol{\epsilon}\boldsymbol{\psi}(\lambda)h(t), \tag{2.24}$$

where

$$h(t) = \begin{pmatrix} -\psi f^{-1} & -t^{-1}f^{-1} \\ t(f + \psi^2 f^{-1}) & \psi f^{-1} \end{pmatrix} \tag{2.25}$$

and $f = \operatorname{Re}\mathscr{E}$, $\psi = \operatorname{Im}\mathscr{E}$, evaluated at $\alpha = 0, \beta = (2t)^{-1}$. The matrix $h(t)$ obeys the relations (A12). In Eq. (2.23), $\tilde{F}(t)$ is the value of the analytic continuation of $F(t)$ on the second Riemann sheet. [The validity of these relations depends on analyticity of $\mathscr{E}(\alpha,\beta)$ at the origin (0,0), which can be brought about by a time translation, $\beta \rightarrow \beta$ + constant (or axial translation, $z \rightarrow z$ + constant, in the stationary case), if $\mathscr{E}$ is analytic at at least one point of the axis.]

Now, use Eq. (2.6a) to eliminate $\boldsymbol{\chi}_1$ in Eqs. (2.8) and (2.9) and replace λ by α^2/λ in the latter: the results are

$$\mathbf{g}' = \boldsymbol{\chi}_2(\alpha^2/\lambda)G(\alpha^2/\lambda)\mathbf{g}\boldsymbol{\chi}_2(\lambda)^T, \tag{2.26a}$$

$$\mathbf{g}' = \boldsymbol{\chi}_2(\alpha^2/\lambda)\mathbf{g}G(\lambda)^T\boldsymbol{\chi}_2(\lambda)^T. \tag{2.26b}$$

Comparison of these two equations gives

$$G(\alpha^2/\lambda)\mathbf{g} = \mathbf{g}G(\lambda)^T. \tag{2.27}$$

Next, use Eqs. (2.6b), (2.14), (2.24), and (B14) and observe that $\mathbf{g}$ and $\boldsymbol{\psi}(\lambda)$ can be cancelled from the final equation [remember that $G_0(t)$ is unaffected by the replacement, $\lambda \rightarrow \alpha^2/\lambda$]. The result is

$$h(t)G_0(t)h(t)^{-1} = G_0(t)^{-1}. \tag{2.28}$$

From Eqs. (A12), this can be written

$$[G_0(t)h(t)]^2 = -I, \tag{2.29}$$

which itself implies

$$\operatorname{tr}[G_0(t)h(t)] = \operatorname{tr}[h(t)G_0(t)] = 0. \tag{2.30}$$

Since the product of a traceless matrix with $\boldsymbol{\epsilon}$ in either order is symmetric and vice versa, it follows that Eq. (2.30) expresses the required symmetry condition on $G_0(t)$.

We are now in a position to establish the exact relationship between the BZ nonsoliton and HE formalisms. Start again with Eq. (2.14a) and use Eqs. (2.7a), (2.6b), (2.24), and (B14) to obtain an equation in which $\mathbf{g}$, $\boldsymbol{\psi}(\lambda)$ and their transforms can be cancelled out. The result is

$$h'(t)G_0(t)h(t)^{-1} = I, \tag{2.31}$$

where $h'(t)$ is calculated from Eq. (2.25) with primed variables. This equation, which can be written

$$h'(t) = h(t)G_0(t)^{-1} = G_0(t)h(t), \tag{2.32}$$

is in fact a formula for the transformed Ernst potential $\mathscr{E}'$ on the axis $\alpha = 0 = \rho$, according to Eq. (2.25). It is an important formula in its own right and, incidentally, shows that $G_0(t)$ is a genuine representation of $\mathscr{K}$ in that the group product is represented by the matrix product. An alternative interpretation of Eq. (2.32) is that it provides a formula for $G_0(t)$ in terms of the initial and final values of the Ernst potential on the axis, thereby demonstrating the transitivity of $\mathscr{K}$ on the space of solutions analytic at and near $(\alpha,\beta) = (0,0)$. Already, Hauser and Ernst have derived just such a formula for their representing matrix $u(t)$[5]:

$$(t\mathscr{E}', \ i)u(t)\begin{pmatrix} -it^{-1} \\ \mathscr{E} \end{pmatrix} = 0, \tag{2.33}$$

where $\mathscr{E}$ and $\mathscr{E}'$ are to be evaluated at $\alpha = 0 = \rho$, $\beta = (2t)^{-1} = z$. Indeed, Eq. (2.33) has already been used in the derivation of Eq. (2.25) in Appendix A.

By expressing $\mathscr{E}'$ as the subject in Eq. (2.33) and separating into real and imaginary parts, we get from Eq. (2.25) the equivalent formula,

$$h'(t) = u(t)h(t)u(t)^{-1}, \tag{2.34}$$

in agreement with Eq. (A15) which was derived directly from the definition (A11) of $h(t)$. Finally, comparison of Eqs. (2.32) and (2.34) reveals the desired relationship between $G_0(t)$ and $u(t)$:

$$G_0(t) = u(t)h(t)u(t)^{-1}h(t)^{-1}. \tag{2.35}$$

Clearly, conditions (2.5), (2.14), and (2.30) [or (2.29)] on $G_0(t)$ are satisfied identically.

Now, if one wishes to calculate the transform of $\mathscr{E}$ and $F(t)$ under an element of $\mathscr{K} \subset \mathrm{K}$ represented by $u(t)$, one can, in principle, substitute Eq. (2.35) into Eqs. (2.6a,b) and solve the BZ homogeneous Hilbert problem. However, a serious difficulty arises with a large class of $u(t)$ matrices for which the HE HHP can be solved explicitly in closed form. These $u(t)$ matrices have only poles and/or quadratic branch points[11] and represent finite products of null generalized[16] HKX transformations[12] and Harrison transformations.[13,14] The HE HHP can be solved without a detailed knowledge of the analytic behavior of $F(\rho,z,t)$ or $\mathscr{E}(\rho,z)$ and the resulting expression for $F'(t)$ is a rational function of $F(t)$ and the values of $F(t)$ and possibly some of its t-derivatives at the singular points of $u(t)$. The same methods will not work for the BZ HHP in its present form because of the appearance of $h(t)$ which depends on the analytic behavior of $\mathscr{E}(0,(2t)^{-1})$ in the complex t plane. In the next paragraph, we provide an alternative formulation of the BZ HHP in which $h(t)$ does not appear.

Substitute Eq. (2.35) into Eqs. (2.6a,b) to give

$$\chi_1(\lambda) = \chi_2(\lambda)\psi(\lambda)u(t)h(t)u(t)^{-1}h(t)^{-1}\psi(\lambda)^{-1}. \tag{2.36}$$

Define

$$Y(\lambda) = \psi'(\lambda)u(t)\psi(\lambda)^{-1}$$
$$= \chi_2(\lambda)\psi(\lambda)u(t)\psi(\lambda)^{-1}. \tag{2.37a}$$

Then, from Eqs. (2.36) and (2.24),

$$Y(\lambda) = \chi_1(\lambda)\mathbf{g}\epsilon\psi(\alpha^2/\lambda)u(t)\psi(\alpha^2/\lambda)^{-1}(\mathbf{g}\epsilon)^{-1}. \tag{2.37b}$$

The new form of the HHP is expressed by equating the right-hand sides of Eqs. (2.37a) and (2.37b). Also, in terms of the matrix function $Y(\lambda)$, the auxiliary relation (2.8) reads

$$\mathbf{g}' = Y(\alpha^2/\lambda)\mathbf{g}Y(\lambda)^T. \tag{2.38}$$

Observe that all the factors in Eq. (2.37a) are analytic in $\Gamma_2 - \{\lambda_2\}$ except $u(t)$ and all the factors in Eq. (2.37b) are analytic in $\Gamma_1 - \{\lambda_1\}$ except $u(t)$. [Conditions (1.13d) and (2.4) guarantee that $Y(\lambda)$ is analytic at both $\lambda = \lambda_1, \lambda_2$.] This fact allows the new HHP to be solved in closed form for the $u(t)$ which have only poles and quadratic branch points as in Ref. 11. [Of course, the HHP (2.6a,b) can be solved by the same methods in a large number of cases where both $F(t)$ and $G_0(t)$ are specified.] In Sec. 3, we derive the Harrison and HKX transformations from the HHP (2.37a,b) by methods comparable to those of Ref. 11, and we also generate the general Weyl (Einstein–Rosen) solution from flat space using the original form (2.6a,b) of the BZ HHP.

The unknowns $X_+(t)$ and $X_-(t)$ in the HE HHP can be expressed in terms of the BZ unknowns $\chi_2(\lambda)$ and $\chi_1(\lambda)$ by the following symmetric relations:

$$X_+(t) = \frac{\lambda}{\alpha^2 - \lambda^2}[-\chi_2(\lambda)(\lambda I - i\mathbf{g}\epsilon)$$
$$+ \chi_1(\alpha^2/\lambda)(\alpha^2\lambda^{-1}I - i\mathbf{g}\epsilon)], \tag{2.39a}$$

$$X_-(t) = \frac{\lambda}{\alpha^2 - \lambda^2}[-Y(\lambda)(\lambda I - i\mathbf{g}\epsilon)$$
$$+ Y(\alpha^2/\lambda)(\alpha^2\lambda^{-1}I - i\mathbf{g}\epsilon)], \tag{2.39b}$$

$\lambda \in \Gamma_2$ in (2.39a), no restriction on λ in (2.39b). These equations show directly that $X_+(t)$ is analytic in the region Γ_2 of the λ plane, and $X_-(t)$ is invariant under the replacement $\lambda \to \alpha^2/\lambda$ and hence is analytic at the branch points of $S(t)$ in the t plane. The inverse relations are

$$\chi_2(\lambda) = \operatorname{Re} X_+(t) - \lambda^{-1}\operatorname{Im} X_+(t)\mathbf{g}\epsilon, \quad \lambda \in \Gamma_2, \tag{2.40a}$$

$$\chi_1(\alpha^2/\lambda) = \operatorname{Re} X_+(t) - (\lambda/\alpha^2)\operatorname{Im} X_+(t)\mathbf{g}\epsilon, \quad \lambda \in \Gamma_2, \tag{2.40b}$$

$$Y(\lambda) = \operatorname{Re} X_-(t) - \lambda^{-1}\operatorname{Im} X_-(t)\mathbf{g}\epsilon, \quad \text{for all } \lambda. \tag{2.40c}$$

These five relations, together with Eq. (2.35), allow the BZ HHP to be deduced from the HE HHP and vice versa. In particular, the auxiliary relations (2.8) and (2.38) are immediate consequences of Eq. (75) of Ref. 4 and vice-versa. Thus the restriction on the gauge of $\psi'(\lambda)$ implied by (2.8) is compatible with the original gauge restrictions on the potentials of Ref. 8. If mixed soliton–nonsoliton transformations are under consideration, $\chi_{1,2}(\lambda)$ and $Y(\lambda)$ in the above formulas should be replaced by $\Delta^{-1/2}\chi_{1,2}(\lambda)$ and $\Delta^{-1/2}Y(\lambda)$, respectively, where Δ is given by Eq. (2.22).

There is an important qualitative difference between the group representations denoted by $u(t)$ and $G_0(t)$. First, $u(t)$ can serve as a representing matrix for an abstract Lie group which exists independently of solutions of Einstein's equations, whereas $G_0(t)$ cannot: condition (2.30) explicitly involves the Ernst potential $\mathscr{E}$ through $h(t)$. Further, since $G_0(t)$ is uniquely determined in terms of the initial and final solutions by Eq. (2.32), it follows that $G_0(t)$ does not faithfully represent the multiple transitivity of the $\mathscr{K}$-group. We can say that $G_0(t)$ faithfully represents a simply transitive factor group in which each element is an equivalence class of members of $\mathscr{K}$ which transform any initial solution to the same final solution. The equivalence class for each $G_0(t)$ can be expressed by solving Eq. (2.35) for $u(t)$: the result is

$$u(t)=G_0(t)^{1/2}\{[\cos\theta(t)]I+[\sin\theta(t)]h(t)\}, \qquad (2.41)$$

where $\theta(t)$ is an arbitrary function of t, real for real t, and analytic in $L+L_-$ and at $t=\infty$, and where

$$G_0(t)^{1/2}=D^{-1/2}[I+G_0(t)], \qquad (2.42a)$$

$$D=\det[I+G_0(t)]=2+\operatorname{tr}G_0(t). \qquad (2.42b)$$

The transformations in $\mathscr{K}$ which preserve asymptotic flatness in the stationary axisymmetric case can be identified from Eq. (2.33) which expresses $\mathscr{E}'(0,z)$ in terms of $\mathscr{E}(0,z)$ and $u(t)$. A simple calculation shows that a *necessary and sufficient condition for preservation of asymptotic flatness* up to a NUT parameter is

$$\begin{pmatrix}1&0\\0&t^{-1}\end{pmatrix}u(t)\begin{pmatrix}1&0\\0&t\end{pmatrix}\text{ is analytic at } t=0. \qquad (2.43a)$$

According to Eqs. (2.35) and (2.25), an equivalent statement is

$$\begin{pmatrix}1&0\\0&t^{-1}\end{pmatrix}G_0(t)\begin{pmatrix}1&0\\0&t\end{pmatrix}\text{ is analytic at } t=0. \qquad (2.43b)$$

The definition of asymptotic flatness assumed here is given in Appendix B of Ref. 16. It must be emphasized how trivially easy it is to identify asymptotic flatness preserving transformations in terms of representing matrices. This powerful feature allows the investigator to work confidently with more general transformations in $\mathscr{K}$ since it is easy to recognize combinations of the latter which preserve asymptotic flatness (e.g., even number of Harrison transformations) and to identify members of $\mathscr{K}$, if any, which map a given asymptotically nonflat solution to an asymptotically flat solution (e.g., single Harrison transform of the "stationary C metric").

3. EXAMPLES

In this section, we investigate the BZ homogeneous Hilbert problem (2.6a, b) or its alternative form (2.37a, b) in four special cases: (A) Harrison's Bäcklund transformation,[13,14,16] (B) the null generalized HKX transformation,[12,16] (C) generation of the general Weyl (Einstein–Rosen) solution from flat space,[9] and (D) generation of the nonlinear superposition of n Kerr–NUT particles from the superposition of n Schwarzschild particles using the **B** group.[10] The first three examples have already been treated in the HE representation (Refs. 11, 3 and 11, and 4, respectively) and it is instructive to compare the calculations. Also, Hauser and Ernst have generated Kerr–NUT from Schwarzschild using their integral-equation representation of the **B** group.[3] In Sec. 3D, we discuss the **B** group from the standpoint of the BZ and HE HHP's and we find that the BZ representation of the n-Schwarzschild→n-Kerr–NUT transformation is different from the others, being of *pure-soliton* type.

A. Harrison's Bäcklund transformation

Let us solve the BZ HHP written in the alternative form of Eqs. (2.37a, b),

$$\psi'(\lambda)u(t)\psi(\lambda)^{-1}$$
$$=\chi_1(\lambda)\mathbf{g}\boldsymbol{\epsilon}\psi(\alpha^2/\lambda)u(t)\psi(\alpha^2/\lambda)^{-1}(\mathbf{g}\boldsymbol{\epsilon})^{-1}, \qquad (3.1)$$

for[11]

$$u(t)=\left(1-\frac{s}{t}\right)^{-1/2}\begin{pmatrix}1&-cst^{-1}\\-c^{-1}&1\end{pmatrix}. \qquad (3.2)$$

The unknowns are $\psi'(\lambda)$ analytic in Γ_2 and obeying condition (2.4) and $\chi_1(\lambda)$ analytic in Γ_1 and obeying condition (2.10). Write

$$(\lambda-\mu_2)(\lambda-\mu_1)=\lambda^2+(2\beta-s^{-1})\lambda+\alpha^2$$
$$=\lambda(st)^{-1}(s-t),$$

with $\mu_2=\mu(s)\in\Gamma_2$, $\mu_1=\nu(s)\in\Gamma_1$. Since $u(t)$ appears linearly and homogeneously in Eq. (3.1), the quadratic surd $(1-s/t)^{-1/2}$ cancels out and so $u(t)$ can be replaced by the rational matrix function,

$$v(t)=\begin{pmatrix}1&-c[1+s\lambda^{-1}(\lambda-\mu_2)(\lambda-\mu_1)]\\-c^{-1}&1\end{pmatrix}, \qquad (3.3)$$

which has poles at $\lambda=0,\infty$ and a vanishing determinant at $\lambda=\mu_2,\mu_1$.

Now, $\psi'(\lambda)v(t)\psi(\lambda)^{-1}$ is analytic throughout Γ_2 (including $\lambda=\lambda_2$ and $\lambda=\mu_2$) except for the origin $\lambda=0$ where it has a simple pole with residue,

$$\mathbf{g}'\begin{pmatrix}0&-cs\alpha^2\\0&0\end{pmatrix}\mathbf{g}^{-1}=cs\begin{pmatrix}f'_{11}\\f'_{12}\end{pmatrix}(f_{12},\ -f_{11}). \qquad (3.4)$$

Similarly, $\chi_1(\lambda)\mathbf{g}\boldsymbol{\epsilon}\psi(\alpha^2/\lambda)v(t)\psi(\alpha^2/\lambda)^{-1}(\mathbf{g}\boldsymbol{\epsilon})^{-1}$ is analytic throughout Γ_1 (including $\lambda=\lambda_1$ and $\lambda=\mu_1$) and grows linearly as $\lambda\to\infty$, say $\sim\mathbf{e}\lambda$, where

$$\mathbf{e}=cs\begin{pmatrix}0&0\\1&0\end{pmatrix}.$$

It follows that

$$\psi'(\lambda)v(t)\psi(\lambda)^{-1}=\chi_1(\lambda)\mathbf{g}\boldsymbol{\epsilon}\psi(\alpha^2/\lambda)v(t)\psi(\alpha^2/\lambda)^{-1}(\mathbf{g}\boldsymbol{\epsilon})^{-1}$$
$$=A\lambda^{-1}+B+cs\lambda\begin{pmatrix}0&0\\1&0\end{pmatrix}\equiv Z(\lambda), \qquad (3.5)$$

where A and B are matrices depending only on (α,β), to be determined.

From Eq. (3.5),

$$\psi'(\lambda)=\frac{\lambda}{s(\lambda-\mu_2)(\lambda-\mu_1)}Z(\lambda)\psi(\lambda)\boldsymbol{\epsilon}v(t)^T\boldsymbol{\epsilon}, \qquad (3.6)$$

$$\chi_1(\lambda)=-\frac{\lambda}{s(\lambda-\mu_2)(\lambda-\mu_1)}Z(\lambda)\mathbf{g}(\psi(\alpha^2/\lambda)^{-1})^T$$
$$\times v(t)^T\psi(\alpha^2/\lambda)^T\mathbf{g}^{-1}, \qquad (3.7)$$

where we have used the identity (B14). The right-hand side of Eq. (3.6) must not have a pole at $\lambda=\mu_2$ in Γ_2 and the right-hand side of Eq. (3.7) must not have a pole at $\lambda=\mu_1$ in Γ_1. Since $v(t)$ is degenerate at $\lambda=\mu_1$ and $\lambda=\mu_2$, the conditions that the respective residues vanish reduce to the following column-vector equations:

$$Z(\mu_2)\psi(\mu_2)\begin{pmatrix}c\\1\end{pmatrix}=0, \qquad (3.8)$$

$$Z(\mu_1)\mathbf{g}\boldsymbol{\epsilon}\psi(\mu_2)\begin{pmatrix}c\\1\end{pmatrix}=0. \qquad (3.9)$$

These equations provide only four equations for the eight unknown entries in A and B. Since A is given by either side of Eq. (3.4), we have

$$A\begin{pmatrix} f_{11} \\ f_{12} \end{pmatrix} = fA\begin{pmatrix} 1 \\ -\omega \end{pmatrix} = 0 \tag{3.10}$$

[recall Eq. (1.4)]. A fourth column-vector equation can be deduced from the requirement $\chi_1(\infty) = I$. Taking the limit as $\lambda \to \infty$ of the right-hand side of Eq. (3.7), we find

$$B\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} c^{-1} \\ 1 \end{pmatrix} + cs\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \mathbf{g}\epsilon\dot{\psi}(0)\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$= \begin{pmatrix} c^{-1} \\ 1 + cs\psi \end{pmatrix}, \tag{3.11}$$

where $\psi = \operatorname{Im} \mathscr{E}$. In deriving Eq. (3.11), we have used Eqs. (B8b), (B5), (A6b), and (1.8).

The solution of Eqs. (3.8)–(3.11) for the matrices A and B is now a straightforward problem in linear algebra. The result, after some rearrangement, is

$$A = \begin{pmatrix} c^{-1}\operatorname{Im} T & 0 \\ \operatorname{Im}[(1 - ics\mathscr{E})T] & csf \end{pmatrix} \mathbf{g}\epsilon + cs\alpha^2\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{3.12a}$$

$$B = \begin{pmatrix} -c^{-1}\operatorname{Re} T & c^{-1} \\ -\operatorname{Re}[(1 - ics\mathscr{E})T] & 1 + cs\psi \end{pmatrix}$$
$$- c(1 - 2s\beta)\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{3.12b}$$

where the complex pseudopotential T is defined by

$$T = T_{(\mathrm{N})}/T_{(\mathrm{D})}, \tag{3.13a}$$

$$\begin{pmatrix} T_{(\mathrm{D})} \\ T_{(\mathrm{N})} \end{pmatrix} = (\mu_1 - \mu_2)^{-1}(I + i\mu_2{}^{-1}\mathbf{g}\epsilon)\boldsymbol{\psi}(\mu_2)\begin{pmatrix} c \\ 1 \end{pmatrix}. \tag{3.13b}$$

Hence, from Eqs. (3.6), (3.5), and (3.3), the solution of the HHP is

$$\boldsymbol{\psi}'(\lambda) = -[s(\lambda - \mu_2)(\lambda - \mu_1)]^{-1}\left\{A + \lambda B + cs\lambda^2\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right\}$$
$$\times \boldsymbol{\psi}(\lambda)\begin{pmatrix} 1 & c[1 + s\lambda^{-1}(\lambda - \mu_2)(\lambda - \mu_1)] \\ c^{-1} & 1 \end{pmatrix}. \tag{3.14}$$

The limiting form of this equation as $\lambda \to 0$ gives the transformed metric

$$\mathbf{g}' = \boldsymbol{\psi}'(0) = \begin{pmatrix} f'_{11} & f'_{12} \\ f'_{12} & f'_{22} \end{pmatrix}, \tag{3.15}$$

where

$$f'_{11} = -(1/c^2 s)\operatorname{Im} T, \tag{3.16a}$$

$$f'_{12} = -(1/cs)\operatorname{Im}[(1 - ics\mathscr{E})T] + f\omega, \tag{3.16b}$$

$$f'_{22} = -(1/s)\operatorname{Im}[(1 - ics\mathscr{E})^2 T] + 2cf\omega(1 + cs\psi)$$
$$+ c^2 f(1 - 2s\beta). \tag{3.16c}$$

It can now be shown directly that Eqs. (2.8) [or (2.38)] and (2.12a, b) are satisfied identically.

It is not difficult to obtain the transformed complex $F(t)$ potential from $\boldsymbol{\psi}'(\lambda)$ and $\mathbf{g}'$. The relevant formulas are in Appendix B. Restrict λ to the open disk Γ_2 so that $\lambda = \mu(t)$, $\mu_2 = \mu(s)$, $\mu_1 = \nu(s)$. We find

$$T_{(\mathrm{N})} = F_{22}(s) + cF_{21}(s), \quad T_{(\mathrm{D})} = F_{12}(s) + cF_{11}(s), \tag{3.17}$$

$$F'(t) = \frac{t}{t - s}\begin{pmatrix} -c^{-1}T & c^{-1} \\ c(s - t)t^{-1} - (1 - ics\mathscr{E})T & 1 - ics\mathscr{E} \end{pmatrix}$$
$$\times F(t)\begin{pmatrix} 1 & cst^{-1} \\ c^{-1} & 1 \end{pmatrix}, \tag{3.18}$$

in exact agreement with Refs. 11 and 16.

The principal difference between the derivation of Eq. (3.18) here for the Harrison transformation and the derivation of the same equation in Ref. 11 [Eq. (3.21)] arises from the fact that each singularity of $u(t)$ or $v(t)$, or degeneracy of $v(t)$, in the t plane corresponds to two singularities in the λ plane, one in Γ_2, the other in Γ_1. Thus the number of unknown coefficients to be determined in the BZ HHP is exactly double the number in the HE HHP. The same comment applies to the product of several Harrison transformations, including confluent cases such as the null HKX transformation which is the product of two Harrison transformations with same s parameters.[11,16] Thus the HE HHP leads to shorter computations in these cases. An additional advantage of the HE formalism is the use of complex potentials which also often lead to shorter expressions.

B. The null HKX transformation

In Ref. 11, we solved the HE HHP for the $u(t)$ given by the following SL(2)-covariant expression,

$$u(t) = u^A{}_B(t) = -\epsilon^A{}_B + [at/(t - s)]q^A q_B, \tag{3.19}$$

where a, s and q^A ($A = 1, 2$) are real constants, a being a canonical group parameter for fixed s and q^A. [In SL(2)-tensor equations, $\epsilon^{AB} = \boldsymbol{\epsilon} = \epsilon_{AB}$ is the index raising and lowering operator, e.g., $q_B = q^X\epsilon_{XB}$, $q^A = \epsilon^{AX}q_X$, and, in particular, $\epsilon_B{}^A = -\epsilon^A{}_B = \delta^A_B$.] The result was the null generalized HKX transformation,[11,16,33]

$$\mathrm{F}'_{AB}(t) = \left\{F_A{}^X(t) + \frac{aq^C q^D F_{AC}(s)[G_D{}^X(s, t) - s(s - t)^{-1}\epsilon_D{}^X]}{1 - aq^E q^F G_{EF}(s, s)}\right\}g_{XB}(t), \tag{3.20}$$

where

$$G_{AB}(s, t) = \frac{s}{s - t}\epsilon_{AB} + \frac{tS(s)}{s - t}F_{XA}(s)F^X{}_B(t), \tag{3.21}$$

$$g_{AB}(t) = u_{BA}(t) \quad \text{or} \quad g(t) = u(t)^{-1} \tag{3.22}$$

[recall $g(t) = -g^A{}_B(t)$, $g_{AB}(t) = \boldsymbol{\epsilon}g(t)$, and Eq. (B14)]. This transformation preserves modified special HE gauge[30] since $u(t)$ is analytic at and near $t = \infty$ but does not satisfy condition (1.13d), except when $q^1 = 0$. The factor $g_{XB}(t)$ on the right-hand side of Eq. (3.20) is a gauge function since $g(t)[= -g^A{}_B(t)]$ satisfies conditions (A8). If this gauge function is deleted [i.e., $g_{XB}(t) = \epsilon_{XB}$ or $g(t) = I$], the resulting transformation is denoted the "extended" HKX transformation.[16] This transformation is of pure-soliton type and the close relationship between certain pure-soliton and pure-nonsoliton transformations is discussed at the end of this subsection.

In order to derive the null HKX transformation (3.20) from the BZ nonsoliton formalism, we must abandon SL(2) covariance and insist on special HE gauge and condition (1.13d). These requirements can be met by multiplying the $u(t)$ of Eq. (3.19) on the left by[30]

$$\mathbf{b}=\begin{pmatrix}1 & -b\\ 0 & 1\end{pmatrix},\quad b=\frac{a(q^1)^2}{1+aq^1q^2}. \tag{3.23}$$

The resulting representing matrix is

$$\bar{u}(t)=\mathbf{b}u(t)=\begin{pmatrix}1-\dfrac{aq^1q^2t}{(1+aq^1q^2)(t-s)} & \dfrac{a(q^1)^2s}{(1+aq^1q^2)(t-s)}\\ -\dfrac{a(q^2)^2t}{t-s} & 1+\dfrac{aq^1q^2t}{t-s}\end{pmatrix}. \tag{3.24}$$

This $\bar{u}(t)$ has a simple pole at $t=s$ and hence, when written as a function of λ, it has simple poles at $\lambda=\mu_2=\mu(s)$ in Γ_2 and $\lambda=\mu_1=\nu(s)$ in Γ_1 as in the preceding subsection.

We take the BZ HHP in the form (2.37a, b) and observe immediately that $Y(\lambda)$ must be analytic everywhere except for simple poles at $\lambda=\mu_2,\mu_1$ only. Thus

$$Y(\lambda)=Y(\infty)\left[I+\frac{C}{\lambda-\mu_2}+\frac{D}{\lambda-\mu_1}\right], \tag{3.25}$$

where C and D are matrix functions of (α,β) to be determined, and, from the boundary condition (2.10),

$$Y(\infty)=-\boldsymbol{\epsilon}\bar{u}(0)\boldsymbol{\epsilon}=(\mathbf{b}^{-1})^T. \tag{3.26}$$

The HHP now reduces to the problem of writing down and solving eight linear equations for the eight unknown entries in C and D.

We shall not show the details of the calculation, but only how the required number of equations can be written down, for thereafter the completion of the calculation is a straightforward problem in linear algebra. [Compare with the calculation of $R_A{}^B$ in Eq. (3.4) of Ref. 11.] First, equate the residues at $\lambda=\mu_2$ on both sides of Eq. (2.37a) and the residues at $\lambda=\mu_1$ on both sides of Eq. (2.37b). We obtain expressions for the matrices C and D in terms of the column vectors

$$\chi_2(\mu_2)\psi(\mu_2)\begin{pmatrix}q^1\\ q^2(1+aq^1q^2)\end{pmatrix},\quad \chi_1(\mu_1)\mathbf{g}\boldsymbol{\epsilon}\psi(\mu_2)\begin{pmatrix}q^1\\ q^2(1+aq^1q^2)\end{pmatrix},$$

respectively. To obtain linear algebraic equations for these column vectors, express $\chi_2(\lambda)$ and $\chi_1(\lambda)$ as the subjects in Eqs. (2.37a, b), respectively, and take the appropriate limits as $\lambda\to\mu_2,\mu_1$, respectively. The final results are

$$C=\frac{a\mu_2}{s(\mu_1-\mu_2)}\frac{1}{m^2+n^2}\,[mI+\mu_2{}^{-1}n\mathbf{g}\boldsymbol{\epsilon}]\psi(\mu_2)\mathbf{q}\mathbf{q}^T\boldsymbol{\epsilon}\psi(\mu_2)^{-1}, \tag{3.27a}$$

$$D=\frac{a}{s(\mu_1-\mu_2)}\frac{1}{m^2+n^2}\,[-nI+\mu_2{}^{-1}m\mathbf{g}\boldsymbol{\epsilon}]\psi(\mu_2)\times\mathbf{q}\mathbf{q}^T\boldsymbol{\epsilon}\psi(\mu_2)^{-1}\mathbf{g}\boldsymbol{\epsilon}, \tag{3.27b}$$

where

$$m=1-\frac{a\mu_2}{s(\mu_1-\mu_2)}\,\mathbf{q}^T\boldsymbol{\epsilon}\psi(\mu_2)^{-1}\dot{\psi}(\mu_2)\mathbf{q}, \tag{3.28a}$$

$$n=-\frac{a}{s(\mu_1-\mu_2)^2}\,\mathbf{q}^T\boldsymbol{\epsilon}\psi(\mu_2)^{-1}\mathbf{g}\boldsymbol{\epsilon}\psi(\mu_2)\mathbf{q}, \tag{3.28b}$$

$$\mathbf{q}=\begin{pmatrix}q^1\\ q^2\end{pmatrix},\quad \mathbf{q}^T\boldsymbol{\epsilon}=(-q^2,q^1). \tag{3.29}$$

This completes the determination of $\psi'(\lambda)$:

$$\psi'(\lambda)=(\mathbf{b}^{-1})^T\left[I+\frac{C}{\lambda-\mu_2}+\frac{D}{\lambda-\mu_1}\right]\psi(\lambda)u(t)^{-1}\mathbf{b}^{-1}. \tag{3.30}$$

Reversal of the trivial transformation represented by Eq. (3.23) yields[30]

$$\psi'(\lambda)=\left[I+\frac{C}{\lambda-\mu_2}+\frac{D}{\lambda-\mu_1}\right]\psi(\lambda)u(t)^{-1}. \tag{3.31}$$

Equation (3.20) for the transform of the complex $F(t)$ potential can now be obtained from Eq. (3.31) by a straightforward application of the formulas of Appendix B [see also Eqs. (6.15)–(6.37) of Ref. 16].

It is instructive to compare this pure-nonsoliton transformation with the pure-soliton "extended" HKX transformation[16] for which

$$\psi'_{\rm ph}(\lambda)=\left[I+\frac{C}{\lambda-\mu_2}+\frac{D}{\lambda-\mu_1}\right]\psi(\lambda), \tag{3.32}$$

and $G_0(t)=I=u(t)$. This is precisely the BZ two-soliton transformation in the limit where the two poles of $\chi_2(\lambda)$ in Γ_2 coalesce to form a double pole at $\lambda=\mu_2$. The quantity in square brackets must now be interpreted as $\Delta^{-1/2}\chi_2(\lambda)$ and so, from Eqs. (2.13b) and (2.22), we have

$$\chi_1(\lambda)=\chi_2(\lambda)=\frac{\lambda-\mu_1}{\lambda-\mu_2}\left[I+\frac{C}{\lambda-\mu_2}+\frac{D}{\lambda-\mu_1}\right]=I+\frac{C+D+(\mu_2-\mu_1)I}{\lambda-\mu_2}+\frac{(\mu_2-\mu_1)C}{(\lambda-\mu_2)^2}. \tag{3.33}$$

We see that the only difference between the pure-soliton and pure-nonsoliton versions of the null HKX transformation is the trivial transformation of Ref. 30 and a different choice of gauge. It is just the singularities of the gauge functions which are manifest in $\Delta^{-1/2}\chi_2(\lambda)$ in Γ_2. The only significant differences appear in the statements of the respective HHP's and the actual details of the derivations: in the pure-nonsoliton case, C and D are uniquely determined from the HHP; in the pure-soliton case, a partial fraction expansion of the form (3.33) is the starting point and C and D are determined by Eq. (2.8) and the differential equations for the $\psi(\lambda)$ potential,[2] aq^Aq^B being the constant of integration. More generally, a similar relationship can be established between the $2n$-fold Harrison transformation with $s=s_1,s_2,\ldots,s_{2n}$ (pure-nonsoliton) and the BZ $2n$-soliton transformation for which $\chi_2(\lambda)$ has poles at $\lambda=\mu(s_1),\mu(s_2),\ldots,\mu(s_{2n})$ in Γ_2. However, $(2n-1)$-soliton BZ transformations contain as a factor the Kramer–Neugebauer involution[18] which is not in $\mathscr{K}$ but may be obtainable as some sort of fanciful limit of pure-nonsoliton transformations in $\mathscr{K}$—see Sec. 4.

The extended HKX transformation can also be derived from a slight modification of the HE formalism which closely parallels the BZ pure-soliton derivation. The representing matrix is

$$u_1(t)=g(t)u(t)=I, \tag{3.34}$$

but the contour L is drawn so that the pole in $u(t)$ and $g(t)$ at

$t=s$ is outside L, i.e., in L_-. The HHP takes the simple form

$$X_-(t)=X_+(t)=F'(t)F(t)^{-1}, \quad X_+(0)=I, \tag{3.35}$$

in which $X_+(t)$ is analytic in L_+ and $X_-(t)$ is analytic in L_- and at $t=\infty$ except for a simple pole at $t=s$. The general solution is

$$F'(t)=\left[I+\frac{stN}{t-s}\right]F(t), \tag{3.36}$$

where N is an arbitrary complex matrix function of (ρ, z). Equation (A7a) shows that N is traceless and degenerate, and Eq. (A7b) leads to a formula for N^* in terms of N. However, to completely determine N up to two constants of integration, it is necessary to substitute Eq. (3.36) into the differential equations (A1) and (A2). Not surprisingly, this is a somewhat lengthier derivation of Eq. (3.20), whether with $g(t)=u(t)^{-1}$ or $g(t)=I$, than the derivations above and in Ref. 11 where the HHP's had unique solutions.

C. Generation of the general Einstein–Rosen or Weyl solution from flat space

Kinnersley and Chitre[9] have shown that the abelian subgroup of **K** generated by the $\gamma_{12}{}^{(k)}$, $k=0, 1, 2, \ldots$, maps flat space to the general Weyl solution

$$\mathscr{E}=f=e^{2\chi}, \quad \chi_{\rho\rho}+\rho^{-1}\chi_\rho+\chi_{zz}=0, \tag{3.37}$$

for which $\chi(\rho, z)$ is analytic at and near $(0, 0)$. More recently, Hauser and Ernst[4] generated the Weyl solution from flat space using their HHP with

$$u(t)=e^{\xi(t)\mathbf{k}}, \quad \mathbf{k}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{3.38}$$

where $\xi(t)$ is analytic in L_-, on L, and at $t=\infty$, and obtained the contour integral expressions, Eqs. (3.47a, b) below. In this subsection, we shall do the corresponding calculation in the BZ formalism and obtain the cylindrical-wave counterpart of the Weyl solution, the Einstein–Rosen solution.[21]

From Eqs. (2.35) and (A22), the BZ representing matrix is

$$G_0(t)=e^{2\xi(t)\mathbf{k}}, \tag{3.39}$$

where now $\xi(t)=\xi(t(\lambda))$ is analytic on and near Γ and at $\lambda=\lambda_{1,2}$. From Eq. (A20) and Appendix B, the $\psi(\lambda)$ potential for flat space is

$$\psi(\lambda)=\begin{pmatrix}1 & 0\\ 0 & \lambda^2+2\beta\lambda+\alpha^2\end{pmatrix}. \tag{3.40}$$

Since $\psi(\lambda)$ commutes with $G_0(t)$, it follows that $G(\lambda)=G_0(t)$. The BZ HHP (2.6a, b) can be reduced to a nonmatrix HHP by the substitutions,

$$\chi_1(\lambda)=\exp[2\eta_1(\lambda)\mathbf{k}], \quad \chi_2(\lambda)=\exp[2\eta_2(\lambda)\mathbf{k}], \tag{3.41}$$

where $\eta_{1,2}(\lambda)$ are nonmatrix functions of α, β, and λ analytic in $\Gamma+\Gamma_{1,2}$, respectively. The HHP takes the form

$$\eta_1(\lambda)=\eta_2(\lambda)+\xi(t(\lambda)), \quad \eta_1(\infty)=0. \tag{3.42}$$

The unique solution is

$$\eta_{1,2}(\lambda)=-\frac{1}{2\pi i}\int_\Gamma \frac{\xi(t(\lambda'))}{\lambda'-\lambda}d\lambda', \quad \lambda\in\Gamma_{1,2}, \tag{3.43}$$

from which we obtain the transformed solution

$$\mathbf{g}'=\exp[2\eta_2(0)\mathbf{k}]\begin{pmatrix}1 & 0\\ 0 & \alpha^2\end{pmatrix}, \tag{3.44a}$$

$$\psi'(\lambda)=\exp[2\eta_2(\lambda)\mathbf{k}]\begin{pmatrix}1 & 0\\ 0 & \lambda^2+2\beta\lambda+\alpha^2\end{pmatrix}. \tag{3.44b}$$

This result is in agreement with Eqs. (3.37) and (A24) written in (α, β) coordinates with

$$\chi=\eta_2(0), \quad \beta(t)=2\eta_2(\lambda)-\eta_2(0). \tag{3.45a,b}$$

Let us now deduce a contour integral for $\beta(t)$ in the cut complex t plane, the branch cut as usual joining the zeros of $S(t)$. First, from Eqs. (3.43) and (3.45b),

$$\begin{aligned}\beta(t)&=-\frac{1}{2\pi i}\int_\Gamma\left[\frac{2}{\lambda'-\lambda}-\frac{1}{\lambda'}\right]\xi(t(\lambda'))d\lambda'\\ &=-\frac{1}{2\pi i}\int_\Gamma\left[\frac{1}{\lambda'-\lambda}-\frac{1}{\lambda'-\alpha^2/\lambda}\right]\xi(t(\lambda'))d\lambda',\\ &\qquad\lambda\in\Gamma_2.\end{aligned} \tag{3.46}$$

Next, deform the circle Γ to a simple closed contour Γ' lying inside Γ such that the annular portion of Γ_2 between Γ' and Γ does not contain any singularities of $\xi(t(\lambda'))$ or the points $\lambda'=\lambda_2$ or $\lambda'=\lambda$. The change of variable $\lambda'=\mu(t')$ maps the contour Γ' to a negatively oriented (clockwise) contour L' in the cut t' plane which encloses the cut itself but no singularities of $\xi(t')$ nor the point $t'=t$. Since the integrand has no residue at $t'=\infty$, the contour L' can be replaced by a positively oriented contour L such that the cut lies in the exterior L_- and all the singularities of $\xi(t')$ and the point $t'=t$ lie in the interior L_+. The result of the transformation is

$$\chi=-\frac{1}{2\pi i}\int_L\frac{\xi(t')}{t'S(t')}dt', \tag{3.47a}$$

$$\beta(t)=-\frac{1}{2\pi i}\int_L\frac{S(t)}{S(t')}\frac{\xi(t')}{t'-t}dt', \quad t\in L_+, \tag{3.47b}$$

in exact agreement with Ref. 4. By differentiating under the integral sign, one can readily show that χ and $\beta(t)/S(t)$ satisfy the cylindrical wave equation and that Eq. (A25) in (α, β) coordinates holds.

D. Generation of the nonlinear superposition of *n* Kerr–NUT particles from *n* Schwarzschild particles using the B group

The **B** group of Kinnersley and Chitre[10] is represented by

$$u(t)=\begin{pmatrix}\cos\theta(t) & t^{-1}\sin\theta(t)\\ -t\sin\theta(t) & \cos\theta(t)\end{pmatrix}, \tag{3.48}$$

where $\theta(t)$ is analytic in $L+L_-$ and at $t=\infty$. It was shown by KC to map flat space to itself, Schwarzschild to Kerr–NUT, and the Zipoy–Voorhees solutions[34] with integer δ-parameter to generalizations of the Tomimatsu–Sato solutions,[35] to be called the KC solutions. Hauser and Ernst have generated Kerr from Schwarzschild using contour integration methods[3] but the same results can be obtained directly from the HE HHP. We shall show that, more generally, the nonlinear superposition of n Kerr–NUT particles ($4n$ parameters: mass, angular momentum, NUT parameter, and position on z axis for each particle) can be generated from the superposition of n Schwarzschild particles ($2n$ parameters) using the HE representation of the **B** group. This is not necessarily the best method of calculation: the general n-Kerr–NUT solution can be generated more easily from flat space by applying $2n$ Harrison transformations[16,28,36] or the BZ $2n$-soliton transformation.[2]

The HE HHP can provide a rational explanation of the fact that the infinite-dimensional **B** group generates only a finite number of arbitrary constants in these cases. First, the $F(t)$ potential of the input Weyl solution (n-Schwarzschild, Zipoy–Voorhees) must *not* be put in special HE gauge, but the unique gauge for which

$$\beta(t)=\beta_{\text{odd}}(t), \tag{3.49}$$

as discussed in Appendix A. [Equation (3.47b) gives $\beta_{\text{odd}}(t)$ when $t\in L_-$, special HE gauge when $t\in L_+$.] The t-plane singularities of $\beta_{\text{odd}}(t)$ all lie in L_-. Second, before specializing the harmonic function χ, a short calculation shows that

$$G(t)\equiv F(t)u(t)F(t)^{-1} \tag{3.50}$$

is even in $S(t)$ and is in fact analytic at the branch points of $S(t)$. The χ-potential for n Schwarzschild particles is the Newtonian potential of n rods with (mass)/(length) $=1/2$ in geometric units and with endpoints at $z=z_i\pm\kappa_i$, $i=1,2,\dots,n$, $\kappa_i>0$, on the z axis. (A Zipoy–Voorhees particle is the limiting case where δ rods coincide.) The formulas for χ and $\beta_{\text{odd}}(t)$ are

$$\chi=\sum_{i=1}^{n}\tfrac{1}{2}\ln\frac{x_i-1}{x_i+1}, \tag{3.51}$$

$$\beta_{\text{odd}}(t)=\sum_{i=1}^{n}\tfrac{1}{2}\ln\frac{x_i(1-2tz_i)-2\kappa_i t y_i-S(t)}{x_i(1-2tz_i)-2\kappa_i t y_i+S(t)}, \tag{3.52}$$

where $(x_i,\ y_i)$ are prolate spheroidal coordinates for each particle defined by

$$\begin{pmatrix}x_i\\ y_i\end{pmatrix}=(2\kappa_i)^{-1}[\rho^2+(z-z_i+\kappa_i)^2]^{1/2}\pm(2\kappa_i)^{-1}[\rho^2+(z-z_i-\kappa_i)^2]^{1/2}, \tag{3.53}$$

positive for x_i, negative for y_i. The key property is that $G(t)$ and $G(t)^{-1}$ are analytic throughout L_- except for simple poles at

$$t=\tfrac{1}{2}(z_i\pm\kappa_i)^{-1}\equiv s_1,s_2,\dots,s_{2n}, \tag{3.54}$$

when these numbers are distinct, and poles of higher multiplicity when there are coincidences.

From Eqs. (1.14) and (3.50),

$$X_+(t)=X_-(t)G(t)^{-1}, \tag{3.55}$$

of which the left-hand side is analytic in L_+ and the right-hand side is analytic in L_- except for the aforementioned poles at $t=s_1,\dots,s_{2n}$. It follows that $X_+(t)$ is a rational function of t of the form, when the s_j are distinct,

$$X_+(t)=F'(t)F(t)^{-1}=I+\sum_{j=1}^{2n}\frac{tA_j}{t-s_j}, \tag{3.56}$$

the A_j being complex matrix functions of (ρ,z) to be determined. When δ of the s_j are equal, a sum of partial fractions appropriate to a pole of order δ should be included in $X_+(t)$. Finally, the requirement of analyticity of $X_-(t)=X_+(t)G(t)$ at the points $t=s_1,\dots,s_{2n}$ in L_- gives $4n$ column-vector equations for the $2n$ unknown matrices A_j, uniquely determining the latter. The final solution does not depend on the detailed behavior of the function $\theta(t)$ but only on the values of $\theta(t)$ at $t=s_1,\dots,s_{2n}$ (and derivatives of orders up to $\delta-1$ when δ of the s_j are equal).

The above discussion will assist us in determining how the **B** group is represented in the BZ formalism. We shall remain in the context of stationary axisymmetric fields. First, since $h(t)$ is given by Eq. (A22) for all Weyl solutions when the gauge obeys Eq. (3.49), it follows from Eqs. (2.35) and (3.48) that

$$G_0(t)=I,\quad \chi_1(\lambda)=\chi_2(\lambda). \tag{3.57}$$

Clearly, the transformation is of *pure-soliton* type. Since the function $\theta(t)$ has disappeared from the problem, the arbitrary constants generated by the transformation will not appear now as values of $\theta(t)$ at $t=s_1,\dots,s_{2n}$ but as integration constants. From Eqs. (2.13b), (2.40a), and (3.56), we see that $\Delta^{-1/2}\chi_2(\lambda)$ has poles at

$$\begin{aligned}\lambda&=\mu(s_1),\dots,\mu(s_{2n})\quad\text{in }\Gamma_2,\\ \lambda&=\nu(s_1),\dots,\nu(s_{2n})\quad\text{in }\Gamma_1,\end{aligned} \tag{3.58}$$

simple if the s_j are distinct, nonsimple otherwise. But $\chi_2(\lambda)$ itself cannot have simple poles in Γ_2 for then $\Delta^{-1/2}\chi_2(\lambda)$ would have quadratic branch points according to Eq. (2.22). Thus $\chi_2(\lambda)$ has *double* poles at $\lambda=\mu(s_1),\dots,\mu(s_{2n})$ in Γ_2 when the s_j are distinct, and poles of double the previous order otherwise. It then follows that $\chi_2(\lambda)$ is analytic throughout Γ_1.

The preceding paragraph identifies the n-Schwarzschild to n-Kerr–NUT transformation as a special case of the $4n$*-soliton transformation* in which the poles of $\chi_2(\lambda)$ in Γ_2 are all of even order. When the s_j are distinct, the full transformation factorizes into $2n$ extended HKX transformations,[16] whose q^A parameters must be chosen appropriately. For example, two of these special extended HKX transformations map Schwarzschild to Kerr–NUT, four map double Schwarzschild to double Kerr–NUT,[37] two of rank zero and two of rank one[12,38] map Zipoy–Voorhees $\delta=2$ to the full KC $\delta=2$ solution.[10]

Only $2n$ of the $4n$ integration constants in the $4n$-soliton transformation can be chosen independently as there are only $2n$ values of $\theta(s_j)$. Also, since the n-Schwarzschild solution is the general *static* $2n$-soliton solution (meaning $2n$-soliton transform of flat space), the general $4n$-soliton transform of the n-Schwarzschild solution with same s-parameters will be a special limiting form of the $6n$-soliton solution or $3n$-Kerr–NUT solution in which the $6n$ s-parameters coincide in threes. This latter solution may be interpreted as the nonlinear superposition of n KC $\delta=3$ particles in which each particle has six of its eight allowed degrees of freedom (including NUT and z position). We need to reduce the six degrees of freedom to four in such a way that each KC $\delta=3$ particle reduces to just a Kerr–NUT particle.

It was claimed in Ref. 16 and will now be proven that n-Schwarzschild transforms into n-Kerr–NUT under $2n$ of the special extended HKX transformations for which

$$q^A = (1, 0) \quad \text{(type I)}, \tag{3.59a}$$

$$\text{or} \quad q^A = (0, 1) \quad \text{(type II)}. \tag{3.59b}$$

(The type I transformations are precisely the original HKX transformations of Ref. 12 and type II can be obtained from type I by interchanging the tensor indices 1 and 2.) A consequence of Eq. (6.46) of Ref. 16 is that these special HKX transformations factorize into two BZ one-soliton transformations of which the first maps static solutions to static and the second maps static to stationary. Let the static-to-static BZ transformations be denoted type I or type II according to the type of the HKX transformations. Since BZ pure-soliton transformations commute exactly, we may perform the $2n$ static-to-static transformations first, choosing the type so as to cancel the Schwarzschild particles one by one and eventually leave flat space. Then the remaining $2n$ static-to-stationary transformations will map flat space to the nonlinear superposition of n Kerr–NUT particles.

The explicit transform of the general Weyl solution under the type I and type II BZ transformations is easily calculated from Eq. (5.19) of Ref. 16. The results are

$$\text{type I BZ:} \quad e^{2\chi'} = \alpha^{-1}\mu(s)e^{2\chi}, \tag{3.60a}$$

$$\text{type II BZ:} \quad e^{2\chi'} = \alpha^{-1}\nu(s)e^{2\chi}, \tag{3.60b}$$

where $\alpha = i\rho$. Consider the case where the Schwarzschild rod singularities are nonoverlapping and take them one at a time. Suppose a given rod connects $z = z_0 - \kappa = (2s_1)^{-1}$ to $z = z_0 + \kappa = (2s_2)^{-1}$ along the z axis, with $\kappa > 0$. Three cases need to be distinguished:

Case 1: $0 < (2s_1)^{-1} < (2s_2)^{-1}$;

Case 2: $(2s_1)^{-1} < 0 < (2s_2)^{-1}$;

Case 3: $(2s_1)^{-1} < (2s_2)^{-1} < 0$.

The correct choice of BZ or HKX type depends on the value of (ρ, z) and the location of the branch cut joining the zeros of $S(t)$ in the t plane. To remove this ambiguity, let the cut intersect the real axis at points $t < \min(s_1,\ldots,s_{2n})$ or $t > \max(s_1,\ldots,s_{2n})$ so that $S(s_j) > 0$ for all j. A straightforward calculation now shows that the selected Schwarzschild rod singularity can be cancelled out by applying the following types of double BZ transformation:

Case 1: type I at $s = s_1$ and type II at $s = s_2$;

Case 2: type II at $s = s_1$ and $s = s_2$;

Case 3: type II at $s = s_1$ and type I at $s = s_2$,

$s = (2z)^{-1}$. The corresponding types of double HKX transformation map the Schwarzschild particle to Kerr–NUT as required rather than to KC $\delta = 3$. The applications of the **B** group in Refs. 3 and 10 belong to *Case 2*. Additional cases can be introduced by changing the sign of some of the x_i in Eq. (3.51) (negative mass particles) and/or replacing some of the x_i by $\pm y_i$.

4. LIMITING TRANSITIONS AND RELAXATION OF BOUNDARY CONDITIONS

We have already remarked that the boundary conditions at $t = \infty$ chosen by Hauser and Ernst are not necessary for the preservation of Einstein's equations, but have the convenient property of guaranteeing uniqueness of the solution of the HHP. For example, there are many transformations in $\mathscr{K}$ represented by $u(t)$ matrices with some sort of singularity at $t = s$, say, in L_+, which have well-defined limits as $s \to \infty$. Simple examples which can be treated by elementary methods are the $s = \infty$ limits of the Harrison and HKX transformations (and products thereof) for which $u(t)$ and/or $X_-(t)$ have, respectively, quadratic branch points and poles at $t = \infty$. Here, we shall discuss the $s = \infty$ null HKX transformation, which preserves asymptotic flatness as for finite s.

A formula for the $s = \infty$ null HKX transform of $F(t)$ can be obtained by simply putting $s = \infty$ in Eq. (3.20). (Actually, in Ref. 16 it was shown by direct exponentiation that the $s = \infty$ *nonnull* HKX transformation is given by essentially the same expression.[39]) The formula can be substantially simplified by observing that the limiting forms of Eqs. (A1) and (A7a,b) imply that

$$F_{AB}(\infty) = F_A h_B, \tag{4.1}$$

where F_A is a complex vector function of (ρ, z) or (α, β) and h_B is a *real constant* vector, in any gauge for which $F_{AB}(t)$ is analytic at $t = \infty$. Similarly, the generating function $G_{AB}(s, t)$ defined by Eq. (3.21) is well defined as either s or t or both tend to infinity, the limiting forms being

$$G_{AB}(s, \infty) = -S(s)F_{XA}(s)F^X h_B, \tag{4.2a}$$

$$G_{AB}(\infty, t) = \epsilon_{AB} + 2tr F_X F^X{}_B(t) h_A, \tag{4.2b}$$

$$G_{AB}(\infty, \infty) = \epsilon_{AB} + G_{BA}(\infty, \infty) = g_A h_B + G h_A h_B, \tag{4.2c}$$

where $r = (\rho^2 + z^2)^{1/2} = (\beta^2 - \alpha^2)^{1/2}$, G is a complex scalar function of (ρ, z) or (α, β), and g_A is any real constant vector satisfying $g_X h^X = 1$ (i.e., $g_1 h_2 - g_2 h_1 = 1$). [We choose a (ρ, z) domain and branch cut so that $S(t)/t \to 2r$ as $t \to \infty$: if the cut is a straight line segment, then $z < 0$ or $\beta < -\alpha$.] From Eqs. (A1) and (A7b), the vector F_A and scalar G satisfy

$$\nabla F_A = -(i/2r^2)[z\nabla H_{AX} + \rho\tilde{\nabla} H_{AX}]F^X, \tag{4.3a}$$

$$\nabla G = F^*{}_X \nabla F^X = (i/2r^3)[(z^2 - \rho^2)\nabla H_{XY} + 2\rho z \tilde{\nabla} H_{XY}]F^X F^Y, \tag{4.3b}$$

$$F^*{}_A = r^{-1}(zF_A + i f_{AX} F^X), \tag{4.4a}$$

$$G^* = G - i r^{-1} f_{XY} F^X F^Y. \tag{4.4b}$$

With the aid of Eqs. (4.1) and (4.2b,c), the limiting form of Eq. (3.20) reduces to

$$F'_{AB}(t) = F_{AB}(t) + 2kt r F_A F_X F^X{}_B(t)/(1 - kG), \tag{4.5}$$

where $k = a(q^X h_X)^2/(1 - a q^X q^Y g_X h_Y)$; k is the only essential parameter. Transformations of the form (4.5) form a one-parameter Lie group and hence iteration does not lead to further transformations.

It is not difficult to deduce from Eq. (4.5) an HHP which admits Eq. (4.5) as a solution. It is more instructive, of course, to see the HHP derived from the limit as $s \to \infty$ of the HHP for the finite-s HKX transformation. For this purpose the form (3.35) of the HHP in which the pole at $t = s$ is *outside* the contour L is more useful. The limiting form of Eq. (3.35) as $s \to \infty$ is

$$X_-(t) = X_+(t) = F'(t)F(t)^{-1}, \quad X_+(0) = I, \tag{4.6}$$

where $X_+(t)$ is analytic in $L + L_+$, $X_-(t)$ is analytic in $L + L_-$, and

$$X_-(t) = O(t) \text{ as } t \to \infty. \tag{4.7}$$

The $u(t)$ matrix is the unit matrix I. The general solution of this HHP is

$$F'_{AB}(t) = (\epsilon_A{}^X - tN_A{}^X)F_{XB}(t), \tag{4.8}$$

where $N_A{}^B$ is an arbitrary complex function of (ρ, z). To identify $N_A{}^B$, it is necessary to go back to the differential and algebraic relations satisfied by $F'(t)$. Equation (A7a) shows that $N_A{}^B$ is null (i.e., $\det N = 0$) and traceless (i.e., $N_{AB} = N_{BA}$) and so we have the factorization, $N_A{}^B = N_A N^B$. From Eqs. (4.1) and (4.8), the condition that $F'_{AB}(t)$ be analytic at $t = \infty$ requires that $N^X F_X = 0$, implying that N_A is proportional to F_A. However, this condition can be relaxed as an $O(t)$ term in $F'_{AB}(t)$ can be absorbed by a change of gauge.

The differential equation (A1) for $F'(t)$ implies that the vector N_A satisfies

$$2z\nabla N_A - 2\rho\tilde{\nabla} N_A = -iN^X\nabla H_{AX} - \tfrac{1}{2}N_A N^X \nabla N_X + N_A \nabla z. \tag{4.9}$$

This equation can be solved by first looking for a particular integral proportional to F_A and comparing with Eqs. (4.3a,b). The particular integral is found to be

$$N_A = [2kr/(1-kG)]^{1/2}F_A, \tag{4.10}$$

where k is a real constant. Substitution of Eq. (4.10) into (4.8) gives the $s = \infty$ HKX transformation (4.5).

This transformation can also be obtained from the pure-nonsoliton part of the BZ formalism by relaxing conditions (2.4) and (2.5). If conditions (2.4) and (2.5) are replaced by the requirements that $\psi(\lambda)$ and $G_0(t)$ be analytic at $\lambda = \lambda_2$, the solution of the BZ HHP remains unique and the resulting transformations are products of elements of $\mathscr{K}$, the $s = \infty$ HKX transformation (4.5), and the unimodular linear transformation of Killing vectors. Consider the BZ HHP in the form (2.37a,b) with

$$u(t) = \mathbf{d} \quad \text{or} \quad u^A{}_B(t) = d^A{}_B, \tag{4.11}$$

$\mathbf{d} = d^A{}_B$ a constant matrix, $\det \mathbf{d} = 1$, and let $\psi(\lambda)$ be in modified special HE gauge,[30] i.e., $\psi(\lambda)$ is analytic in $\Gamma + \Gamma_2$ and $\psi_{AB}(\lambda_2) = 2r(\mathrm{Re}\, F_A)h_B$. The solution of the HE HHP with $u^A{}_B(t) = d^A{}_B$ is simply a rotation of Killing vectors[11]:

$$f'_{AB} = d_A{}^X d_B{}^Y f_{XY}, \quad F'_{AB}(t) = d_A{}^X d_B{}^Y F_{XY}(t) \tag{4.12}$$

(note $d_A{}^B = \boldsymbol{\epsilon}\, \mathbf{d}\, \boldsymbol{\epsilon}$). The method of solution of the BZ HHP follows almost exactly the same lines as in Sec. 3B, so it is not necessary to show details. The final result is found to be

$$F'_{AB}(t) = d_A{}^X d_B{}^Y \left[F_{XY}(t) - \frac{2ntrF_X F_Z F^Z{}_Y(t)}{m + nG} \right], \tag{4.13}$$

where

$$m = d^X{}_Y h_X g^Y, \quad n = d^X{}_Y h_X h^Y. \tag{4.14}$$

The transformation (4.13) is clearly the product of the transformations (4.5) with $k = -n/m$ and (4.12). The factor (4.12) can be chosen to be the simple translation of Footnote 30, but not the identity transformation for then n would be zero.

The general solution of Eq. (4.9) leads to a two-parameter enlargement of the $s = \infty$ HKX transformation. First, by considering gauge changes in $F(t)$ with $g(t) = O(t)$ as $t \to \infty$, the general solution of Eq. (4.3a) can be shown to be

$$F_A^{(\text{gen})} = aF_A + bF^{(1)}{}_A{}^X h_X, \tag{4.15a}$$

a, b real constants, where $F_{AB}^{(1)}$, $F_{AB}^{(2)}$,..., are the coefficients in the descending power series,

$$F_{AB}(t) = F_A h_B + t^{-1}F_{AB}^{(1)} + t^{-2}F_{AB}^{(2)} + \cdots,$$

which converges for $|t| > (2r)^{-1}$ in modified special HE gauge. [Equations (A1) and (A7a,b) lead to differential and algebraic equations for the $F_{AB}^{(n)}$ and Eqs. (4.2a,b,c) imply $2rF^X F_{XB}^{(1)} = -g_B - Gh_B$.] Substituting $F_A^{(\text{gen})}$ for F_A in the right-hand side of Eq. (4.3b) and integrating gives

$$G^{(\text{gen})} = a^2 G + 2abr[F_X h_Y F^{(2)XY} - \det F^{(1)}] + 2b^2 r h_X h_Y F^{(1)}{}_Z{}^X F^{(2)ZY}. \tag{4.15b}$$

The general solution of Eq. (4.9) is now

$$N_A = \left(\frac{2r}{1 - G^{(\text{gen})}} \right)^{1/2} F_A^{(\text{gen})}, \tag{4.16}$$

and the enlarged $s = \infty$ HKX transformation takes the form

$$F'_{AB}(t) = F_{AB}(t) + \frac{2trF_A^{(\text{gen})}F_X^{(\text{gen})}F^X{}_B(t)}{1 - G^{(\text{gen})}}, \tag{4.17}$$

reducing to (4.5) when $a^2 = k$, $b = 0$. This transformation preserves asymptotic flatness and, in particular, maps flat space to extreme Kerr–NUT.

The transformation (4.17) cannot be iterated as it stands because $F'(t) = O(t)$ as $t \to \infty$. This can be repaired by the gauge change,

$$F''_{AB}(t) = F'_A{}^X(t) g_{XB}(t), \quad g_{AB}(t) = \epsilon_{AB} + (b/a)th_A h_B. \tag{4.18}$$

The limit as $t \to \infty$ now gives

$$F''_A = \frac{a^{-1}F_A^{(\text{gen})}}{1 - G^{(\text{gen})}}, \quad G'' = \frac{a^{-2}G^{(\text{gen})}}{1 - G^{(\text{gen})}}, \tag{4.19a,b}$$

$$h''_A = h_A + a^2 g_A, \quad g''_A = g_A. \tag{4.19c,d}$$

The combined transformation given by Eqs. (4.17) and (4.18) satisfies the HHP,

$$X_-(t) = F''(t)u(t)F(t)^{-1}, \tag{4.20}$$

$X_-(t)$ analytic in $L + L_-$, $F''(t)$ analytic in $L + L_+$, with

$$u(t) = u^A{}_B(t) = -\epsilon^A{}_B + (b/a)th^A h_B, \tag{4.21}$$

and boundary conditions

$$X_-(t) = O(t), \quad F''(t) = O(1) \text{ as } t \to \infty, \tag{4.22}$$

and, as usual, $F''_{AB}(0) = i\epsilon_{AB}$. These transformations can be iterated and do not close to form a finite-dimensional Lie group but span an infinite-dimensional subgroup of $\mathbf{K}$ outside $\mathscr{K}$ which preserves asymptotic flatness. The product of n such transformations satisfies an HHP of the form (4.20) with

$$u(t) = O(t^n), \quad X_-(t) = O(t^n), \quad F''(t) = O(1) \tag{4.23}$$

as $t \to \infty$, and with $u(t)$ a matrix polynomial in t of degree n. If

$u(t)$ also has singularities in L_+, then the solution of the HHP is the product of an element of $\mathscr{K}$ and n transformations (4.17)–(4.18).

The Harrison transformation also has a well-defined limit as $s\to\infty$, namely

$$F'(t)=\begin{pmatrix} T & -1 \\ -t^{-1}-i\mathscr{E}T & i\mathscr{E}\end{pmatrix}F(t)\begin{pmatrix} -(h_2/h_1)t & 1 \\ t & 0\end{pmatrix}, \tag{4.24a}$$

where $T=F_2/F_1$, and can be enlarged to have one continuous parameter (b/a) by taking

$$T=F_2^{(\text{gen})}/F_1^{(\text{gen})}. \tag{4.24b}$$

It is a trivial matter to write down an HHP for this transformation in which

$$u(t)=O(t^{1/2}),\quad X_-(t)=O(t^{1/2}), \tag{4.25}$$

as $t\to\infty$, the branch cut joining $t=0$ to $t=\infty$. In Eq. (4.24a), we have deliberately chosen a gauge such that the $s=\infty$ Harrison transformation can be iterated. The product of two of the transformations (4.24) is identical to the transformation (4.17)–(4.18) up to a translation $\omega\to\omega+\text{constant}$.[30]

There is an important discrete involution due to Kramer and Neugebauer[18] which plays a major role in the theory of the Geroch group and Bäcklund transformations[16,28] but which lays outside all existing representations of $\mathbf{K}$. This transformation, to be denoted (I), has the effect,

$$f'=\rho f^{-1},\quad \omega'=j\psi, \tag{4.26a,b}$$

$$\psi'=-j\omega,\quad \mathscr{E}'=\rho f^{-1}-ij\omega, \tag{4.26c,d}$$

where $j=\surd(-1)$ and the symbols are defined by Eqs. (1.4) and (1.8). [The complex conjugation operation of Eq. (A7b) does not apply to j, i.e., $i^*=-i, j^*=j$.] A natural question to ask is whether (I) can be obtained as some suitably defined limit of a sequence of elements of $\mathscr{K}$ as in the preceding paragraphs. Such a limit, if it exists, would be rather contrived and probably not have much practical utility. We shall conclude this paper by presenting an HHP for (I) and a one-parameter family of limiting transitions which work for Weyl solutions but not for stationary solutions.

In Ref. 16, the (I)-transform of $F(t)$ was calculated by first calculating the transforms of $F(t)$ under $\mathbf{Q}$[14,16,40] and $\tilde{\mathbf{Q}}=(I)\mathbf{Q}(I)$ with the aid of Neugebauer's commutation theorem[28] and the KC recurrence relations.[8] Using Eq. (A7b), the result can be written,

$$F'(t)=(1-2tz+2jt\rho)^{-1/2}\left[jt^{-1}\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}+A\right]\times F(t)\begin{pmatrix}0 & 1\\ jt & 0\end{pmatrix}, \tag{4.27a}$$

where

$$A=\begin{pmatrix} ij\mathscr{E}' & -1 \\ \mathscr{E}\mathscr{E}'-2(\rho+jz) & -ij\mathscr{E}\end{pmatrix} \tag{4.27b}$$

and $\mathscr{E}'$ is given by Eq. (4.26d). The (I)-transform of $F^*(t)$ can be deduced by taking the i-complex conjugate of both sides of Eqs. (4.27a,b). If $F(t)$ is in special HE gauge, then $F'(t)$ is analytic in the whole complex t plane except for quadratic branch points of index $-\frac{1}{2}$ at the two zeros of $S(t)$ *as well as at* $t=\infty$, necessitating two cuts. This is an optimum choice of gauge in this case as one of the conditions for the existence of special HE gauge [namely, $f'\neq 0$ on z axis near (0, 0)] is not met; in fact $f'(\rho,z)=O(\rho)$ as $\rho\to 0$ for all points on the axis at which the original solution is nonsingular.

The right-hand side of

$$X_-(t)=(1-2tz+2jt\rho)^{1/2}F'(t)\begin{pmatrix}0 & -jt^{-1}\\ 1 & 0\end{pmatrix}F(t)^{-1} \tag{4.28}$$

is analytic in L_- and at $t=\infty$ and so Eq. (4.28) may be regarded as an HHP for the unknowns $X_-(t)$ and $F'(t)$. (It can be interpreted in one complex dimension by writing $j=-\epsilon i$, $\epsilon=\pm 1$, and later replacing ϵ by ij.) With the boundary conditions (A6a,b) on $F'(t)$ supplemented by either Eq. (A7a) or the relation $H'_{12}-H'_{21}=2iz$, the solution (4.27) is unique except that $\mathscr{E}'$ is an undetermined function of (ρ,z). Equation (4.26d) for $\mathscr{E}'$ can then be deduced from either Eq. (A2) or (A7b).

Equation (4.28) suggests that a suitable candidate for the representing matrix of the (I) transformation is

$$u_0(t)=(-jt)^{1/2}\begin{pmatrix}0 & -jt^{-1}\\ 1 & 0\end{pmatrix}. \tag{4.29}$$

This conclusion is reinforced by the fact that if an element $g\in\mathbf{K}$ is represented by $u(t)$ and its dual element $\tilde{g}=(I)g(I)$ by $\tilde{u}(t)$, then

$$\tilde{u}(t)=u_0(t)u(t)u_0(t). \tag{4.30}$$

Equation (4.30) can be proved without difficulty from Eqs. (3.19a,b,c) of Ref. 16 which relate the infinitesimal $\gamma_{AB}^{(k)}$ transformations[8] to their duals and Eqs. (4.4)–(4.6) of Ref. 11 which relate the $\gamma_{AB}^{(k)}$ to their representing matrices. Furthermore, the representing matrix of the BZ one-soliton transformation can be calculated by multiplying the $u(t)$ matrices of the respective factors in Eq. (5.28) of Ref. 16 [Harrison transformation; (I) transformation; translation, scaling, and gauge transformations] and the result is, perhaps not surprisingly, the unit matrix.

Let (J) denote the product of the involution $\mathscr{E}\to\mathscr{E}^{-1}$ (gravitational duality rotation through π radians) and the (I) transformation. Since (J) has the effect, $e^{2\chi'}=\rho e^{2\chi}$, on the general Weyl solution, $\mathscr{E}=e^{2\chi}$, it follows that if $(J)\in\mathbf{K}$, then (J) must be in some analytic extension of the subgroup of $\mathscr{K}$ represented by Eq. (3.38). The effect of the subgroup (3.38) on Weyl solutions is the linear superposition,

$$e^{2\chi'}=e^{2\bar{\chi}+2\chi},\quad e^{2\beta'(t)}=e^{2\bar{\beta}(t)+2\beta(t)}, \tag{4.31}$$

where $\bar{\chi}$ and $\bar{\beta}(t)$ are given by the right-hand sides of Eqs. (3.47a,b) with $\xi(t)=-\bar{\chi}(0,(2t)^{-1})$; note that $e^{2\bar{\chi}(\rho,z)}$ is analytic and nonvanishing at and near the origin. The (J) transformation represents a linear superposition of χ with the potential of an infinite cylindrical bar of line density $\frac{1}{4}$ (recall that the Schwarzschild "rod" has line density $\frac{1}{2}$). If a piece of the bar containing the origin is removed, say $z_0-\kappa<z<z_0+\kappa$, then the superposition is of the form (4.31) with

$$e^{2\bar{\chi}}=\kappa(x+1)(1-y^2)^{1/2}, \tag{4.32}$$

where the (x,y) are prolate spheroidal coordinates [see Eq.

(3.53) with $z_i = z_0$ and subscript i dropped] and is represented by

$$u(t) = \begin{pmatrix} \sigma^{-1}(t) & 0 \\ 0 & \sigma(t) \end{pmatrix}, \quad \sigma(t) = [4\kappa^2 - t^{-2}(1 - 2tz_0)^2]^{1/4}. \tag{4.33}$$

Let this transformation be denoted (J_κ); $(J_\kappa) \in \mathscr{K}$ when $\kappa > |z_0|$. Now fix (ρ, z) and z_0 and let κ decrease to $|z_0|$ and thence to zero: we find $e^{2\bar{\chi}} \to \rho$ and so $(J_\kappa) \to (J)$ as $\kappa \to 0$ when applied to Weyl solutions.

The (J_κ)-transform of a generic stationary solution also has a well-defined unambiguous limit as $\kappa \to 0$. The limit, however, depends on z_0 and is *different* from the (J)-transform for all z_0. To prove this statement, it is sufficient to exhibit a single counterexample. Now the (J_κ)-transform of a slowly rotating solution,

$$\mathscr{E} = e^{2\chi} + i\epsilon\psi + O(\epsilon^2), \tag{4.34a}$$

$$\nabla_3{}^2\chi = 0, \quad \nabla_3{}^2\psi - 4\nabla\chi\cdot\nabla\psi = 0, \tag{4.34b}$$

ϵ small, can be calculated explicitly by contour integration. First, contour integral expressions for $\psi(\rho, z)$ and, more generally, $F(\rho, z, t)$ analogous to Eqs. (3.47a,b) can be written in terms of $\chi(0, z)$ and $\psi(0, z)$, assumed to be analytic at and near $z = 0$. Equation (2.33) provides an infinity of $u(t)$ matrices of the form $u(t) = I + \epsilon v(t)$ which map $\mathscr{E}_{\text{Weyl}} = e^{2\chi}$ to $\mathscr{E} = e^{2\chi} + i\epsilon\psi$. Then, to first order in ϵ, the multiplicative HHP (1.14) reduces to an additive boundary value problem solvable by standard methods. The final results are

$$F(t) = [I + \epsilon Y_+(t)]F_{\text{Weyl}}(t), \tag{4.35a}$$

$$H = H_{\text{Weyl}} + i\epsilon \dot{Y}_+(0)\epsilon, \tag{4.35b}$$

$$\psi = -\dot{Y}_+(0)_{12}, \tag{4.35c}$$

where

$$Y_+(t) = -\frac{1}{2\pi i}\int_L \frac{t}{s-t}\frac{\psi(0, (2s)^{-1})e^{-2\beta(s)}}{S(s)} \times \begin{pmatrix} i\mu(s) & e^{2\chi} \\ \mu^2(s)e^{-2\chi} & -i\mu(s) \end{pmatrix} ds \tag{4.36}$$

for t in L_+. In these equations, $F_{\text{Weyl}}(t)$ is given by Eq. (A24), H and H_{Weyl} by Eq. (A6b), χ and $\beta(t)$ by Eqs. (3.47a,b), $\mu(t)$ by Eq. (B3a), and the contour L encloses all the singularities of $\psi(0, (2s)^{-1})$.

The (J_κ)-transform of the slowly rotating solution (4.34) is also given by Eqs. (4.35) and (4.36) with χ, $\beta(t)$, ψ, etc., replaced by primed variables, χ', $\beta'(t)$, ψ', etc., calculated from Eqs. (4.31), (4.32), and

$$\psi'(0, (2s)^{-1}) = \sigma^2(s)\psi(0, (2s)^{-1}). \tag{4.37}$$

When $\kappa > |z_0|$, the contour L encloses the two branch points of $\sigma^2(s)$ at $s = \frac{1}{2}(z_0 \pm \kappa)^{-1}$ and the cut joining them, to be denoted C_1 (without loss of generality, take $z_0 > 0$). The cut C_2, joining the zeros of $S(s)$, crosses the real axis on either side of C_1. To understand how $Y'_+(t)$ varies as κ decreases to z_0 and beyond, view the complex s plane in the Riemann sphere topology. When $\kappa < z_0$, the cut C_1 occupies the two semi-infinite portions, $-\infty < s \leqslant \frac{1}{2}(z_0 + \kappa)^{-1}$, $\frac{1}{2}(z_0 - \kappa)^{-1} \leqslant s < \infty$, of the real axis, and C_2 passes between. The contour L takes the form of two open infinite arcs enclosing the two parts of C_1 in the positive sense, as well as the point t and all the singularities of $\psi(0, (2s)^{-1})$, and may be deformed to a clockwise contour L' enclosing only the cut C_2 (as in Sec. 3C). As $\kappa \to 0$, L (or L') and C_2 are pinched off at $s = (2z_0)^{-1}$ as the two ends of C_1 close up the gap, and the integral takes the limiting form

$$Y'_+(t) = \frac{1}{2\pi}\int_{L''} \frac{t}{s-t}\frac{\psi(0, (2s)^{-1})e^{-2\beta(s)}}{S(s)} \times \begin{pmatrix} -i\rho & \nu(s)e^{2\chi} \\ -\mu(s)e^{-2\chi} & i\rho \end{pmatrix} ds, \tag{4.38}$$

where L'' is a "figure-eight" shaped contour which crosses itself at $s = (2z_0)^{-1}$ and encloses C_2, Im $s > 0$, in the positive direction and C_2, Im $s < 0$, in the negative direction.

As an application of Eq. (4.38), the simple solution

$$\mathscr{E} = 1 + i\psi_0, \quad \omega = 0, \tag{4.39}$$

ψ_0 small constant, transforms under (J_κ) in the limit as $\kappa \to 0$ to

$$\mathscr{E}' = \rho + 2i\pi^{-1}\psi_0 r, \quad \omega' = \pi^{-1}\psi_0 \ln\frac{1-\cos\theta}{1+\cos\theta}, \tag{4.40}$$

to order ψ_0, where the spherical coordinates (r, θ) are defined by $\rho = r\sin\theta$, $z - z_0 = r\cos\theta$. For each z_0, this is different from the (J)-transform, which is simply $\mathscr{E}' = 1$, $\omega' = -j\psi_0$. Equations (4.38) and (4.40) also hold when $z_0 \leqslant 0$ [in the case $z_0 = 0$, the cut C_2 joins $s = \frac{1}{2}(z - i\rho)^{-1}$ to $i\infty$ and $\frac{1}{2}(z + i\rho)^{-1}$ to $-i\infty$ and L'' consists of two infinite lines crossing the plane from left to right, one enclosing C_2, Im $s > 0$, in the positive sense, the other enclosing C_2, Im $s < 0$, in the negative sense]. The limits as $z_0 \to \pm\infty$ are also well defined if one compensates unbounded terms by additive constants in ω' and ψ' and by suitably adjusting the gauge of $F'(t)$. Under this latter limit, the transform of (4.39) becomes

$$\mathscr{E}' = \rho \mp 2i\pi^{-1}\psi_0 z, \quad \omega' = \mp 2\pi^{-1}\psi_0 \ln\rho. \tag{4.41}$$

A somewhat different limiting transition can be carried out by superposing a finite rod of length 2κ and line density $\frac{1}{4}$, $e^{2\bar{\chi}} = 2\kappa[(x-1)/(x+1)]^{1/2}$ (Zipoy–Voorhees $\delta = \frac{1}{2}$ particle), and letting $\kappa \to \infty$ with the midpoint fixed at $z = z_0$. In this case, the limiting procedure involves rather lengthy and difficult asymptotic techniques and it is necessary to adjust gauge and admit the translation $\omega \to \omega +$ constant in order to absorb terms of order $\ln\kappa$ in $F'(t)$. The limiting transform of the solution (4.39) turns out to be (4.41) (upper sign if $z_0 < 0$, lower if $z_0 > 0$).

The limiting transitions discussed in the preceding paragraphs do not succeed in obtaining the Kramer–Neugebauer involution (I) as the limit of some sequence of members of $\mathscr{K}$. At this stage, the question of whether or not (I) is in some analytic continuation of $\mathscr{K}$ (and therefore in **K** by definition) remains open. Nevertheless, the foregoing calculations are instructive in that they show for the first time how large classes of solutions involving logarithmic singularities along the entire z axis can be generated from flat space using the Geroch group.

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APPENDIX A: ANALYTIC CONTINUATION OF $F(t)$ ONTO THE SECOND RIEMANN SHEET

The complex matrix potential $F(t)$ $[=F_{AB}(t)=F_{AB}(\rho,z,t)]$ of Kinnersley and Chitre[9,10] (KC) satisfies the two partial differential equations

$$\nabla F(t)=\frac{it}{S^2(t)}\,[(1-2tz)\nabla H-2t\rho\tilde{\nabla}H\,]\epsilon F(t), \quad \text{(A1)}$$

$\nabla=(\partial/\partial\rho,\partial/\partial z)$, $\tilde{\nabla}=(\partial/\partial z,\,-\partial/\partial\rho)$, whose compatibility is guaranteed by the differential equations for the matrix potential $H\,[=H_{AB}=H_{AB}(\rho,z)]$,[7,8]

$$\nabla H=i\rho^{-1}\mathbf{g}\epsilon\tilde{\nabla}H. \quad \text{(A2)}$$

In Eqs. (A1) and (A2) we have used the notation,

$$S(t)=[(1-2tz)^2+4t^2\rho^2]^{1/2}$$
$$=[(1-2t\beta)^2-4t^2\alpha^2]^{1/2},\quad S(0)=1, \quad \text{(A3)}$$

$$\epsilon=\begin{pmatrix}0&1\\-1&0\end{pmatrix}, \quad \text{(A4)}$$

and $\mathbf{g}=\mathrm{Re}\,H$ is the 2×2 block of the metric [see Eqs. (1.1)–(1.5)]. If cylindrically symmetric gravitational wave solutions rather than axially symmetric stationary solutions are under consideration, one should replace the coordinates (ρ,z) by (α,β), where $\alpha=i\rho$, $\beta=z$, and perform the necessary analytic continuations.

If $F_0(t)$ is a particular solution of Eq. (A1) for given $\mathbf{g}=\mathrm{Re}\,H$, the general solution is

$$F(t)=F_0(t)g(t), \quad \text{(A5)}$$

where $g(t)$ is a rational matrix function of t only, not of ρ or z. Since some of the freedom in $F(t)$ is used up by the initial conditions,

$$F(0)=i\epsilon,\quad \dot{F}(0)=H, \quad \text{(A6a,b)}$$

and first integrals,

$$\det F(t)=-1/S(t), \quad \text{(A7a)}$$

$$S(t)F^*(t)=2it\mathbf{g}\epsilon F(t)-(1-2tz)F(t), \quad \text{(A7b)}$$

$F^*(t)$ being the complex conjugate of $F(t^*)$, $g(t)$ is accordingly restricted to obey

$$g(0)=I,\quad \det g(t)=1,\quad g^*(t)=g(t). \quad \text{(A8)}$$

This nonuniqueness in the definition of $F(t)$ gives rise to the infinite-dimensional group of gauge transformations[6,9] acting on the hierarchy of KC potentials [coefficients in the power series expansion (1.9)] which leave invariant the metric $\mathbf{g}=\mathrm{Re}\,H$.

Hauser and Ernst[5] have proved that, under general circumstances, there exists a unique gauge (denoted here "special HE gauge") such that $F(t)$ is analytic in the whole complex t plane except for quadratic branch points at the two zeros of $S(t)$ joined by a cut and that $F(t)\begin{pmatrix}1&0\\0&t\end{pmatrix}$ is analytic at $t=\infty$. Furthermore, the two branch points are of index $-\frac{1}{2}$ in such a way that

$$F(t)=A(t)+B(t)/S(t), \quad \text{(A9)}$$

where $A(t)$ and $B(t)$ are analytic at the zeros of $S(t)$, but will in general have (ρ,z)-independent singularities elsewhere. The principal condition in Hauser and Ernst's theorem is that $F(t)$ be evaluated in an open (ρ,z) domain containing the origin (0, 0) for which $\mathscr{E}=H_{11}$ is an analytic function of ρ and z and $f=\mathrm{Re}\,\mathscr{E}\neq0$ [see Ref. 5 for a detailed discussion of the analyticity properties of $\mathscr{E}(\rho,z)$ and $F(\rho,z,t)$].

In this appendix, we wish to give an explicit determination of the matrix functions $A(t)$ and $B(t)$ in Eq. (A9), or, equivalently, a formula in terms of $F(t)$ for

$$\tilde{F}(t)=A(t)-B(t)/S(t). \quad \text{(A10)}$$

$\tilde{F}(t)$ is simply the result of analytically continuing $F(t)$ across the branch cut and onto the second Riemann sheet. This two-sheeted Riemann surface will not necessarily be the whole Riemann surface for the maximally extended function $F(t)$ because of possible (ρ,z)-independent branch points in $\tilde{F}(t)$ on the second sheet. Since the differential equation (A1) is even in $S(t)$, it follows that $\tilde{F}(t)$ also satisfies Eq. (A1) and so

$$\tilde{F}(t)=iF(t)h(t), \quad \text{(A11)}$$

where $h(t)$ is some matrix function of t only, to be determined (the imaginary unit i is introduced for later convenience). The inverse relation, $F(t)=i\tilde{F}(t)h(t)$, and Eqs. (A7a,b) give the following constraints on $h(t)$:

$$\det h(t)=1,\quad h(t)^2=-I,$$
$$\mathrm{tr}\,h(t)=0,\quad h^*(t)=h(t) \quad \text{(A12)}$$

[cf. Eqs. (6.53) and (6.54) of Ref. 16]. These relations hold for any choice of gauge for $F(t)$.

The determination of $h(t)$ in terms of the Ernst potential $\mathscr{E}$ invokes some of the main results of Ref. 5. First, since special HE gauge is unique when it exists,[5] it follows that, in this gauge, $h(t)$ is uniquely determined in terms of $\mathscr{E}$. (It will be seen that the converse is also true.) First, let us use the homogeneous Hilbert problem (HHP) to find how $h(t)$ transforms under an element of the Geroch group represented by $u(t)$. With a prime denoting transformed variables, the HHP reads,

$$X_-(t)=F'(t)u(t)F(t)^{-1}, \quad \text{(A13)}$$

where $X_-(t)$ is analytic in L_- (the exterior of L) and at $t=\infty$, $F'(t)$ and $F(t)$ are analytic in L_+ (the interior of L). On the second Riemann sheet, we must have

$$X_-(t)=\tilde{F}'(t)u(t)\tilde{F}(t)^{-1}$$
$$=F'(t)h'(t)u(t)h(t)^{-1}F(t)^{-1}, \quad \text{(A14)}$$

since neither $X_-(t)$ nor $u(t)$ can have branch points at the zeros of $S(t)$ in L_-. Comparison of Eq. (A14) with (A13) shows that

$$h'(t)=u(t)h(t)u(t)^{-1}. \quad \text{(A15)}$$

This derivation does not presuppose that either $F(t)$ or $F'(t)$ is in special HE gauge. If both are in the special gauge, $u(t)$ is necessarily analytic in L_- and obeys the HE boundary condition at $t=\infty$ [see Eq. (1.13d)].[5] It is obvious from Eqs. (A5) and (A11) that an arbitrary gauge change,

$$F(t)\mapsto F(t)g(t), \quad \text{(A16a)}$$

has the effect

$$h(t)\mapsto g(t)^{-1}h(t)g(t). \quad \text{(A16b)}$$

The next step is to find all $u(t)$ analytic in L_- which map flat space $\mathscr{E}=1$ to a given stationary solution

$\mathscr{E}' = \mathscr{E}'(\rho, z)$, preserving special HE gauge. It will be necessary that $\mathscr{E}'$ be analytic in a (ρ, z) domain containing the origin (0, 0). The following formula of Hauser and Ernst[5] gives implicitly all group elements $u(t)$ which map any given initial solution $\mathscr{E}$ to any given final solution $\mathscr{E}'$ preserving special HE gauge:

$$(t\mathscr{E}', i)u(t)\begin{pmatrix} -it^{-1} \\ \mathscr{E} \end{pmatrix} = 0, \tag{A17}$$

where $\mathscr{E}$ and $\mathscr{E}'$ are to be evaluated at $\rho = 0, z = (2t)^{-1}$. The real and imaginary parts of this equation, together with the determinant condition (1.13a), provide three equations for the four components of $u(t)$. Now put $\mathscr{E} = 1$ and

$$\mathscr{E}' = f + i\psi = f(0, (2t)^{-1}) + i\psi(0, (2t)^{-1}) \tag{A18}$$

in Eq. (A17) and solve for the components of $u(t)$ in terms of f, ψ, and one arbitrary function of t (hereafter we drop the prime on $\mathscr{E}'$). The result is

$$u(t) = \begin{pmatrix} f^{-1/2} & 0 \\ -t\psi f^{-1/2} & f^{1/2} \end{pmatrix}\begin{pmatrix} \cos\theta(t) & t^{-1}\sin\theta(t) \\ -t\sin\theta(t) & \cos\theta(t) \end{pmatrix}, \tag{A19}$$

where $\theta(t)$ is analytic in L_- and at $t = \infty$, but otherwise arbitrary. The matrix on the right in Eq. (A19) represents the general **B**-group element[10] which maps flat space to itself, preserving special HE gauge. This result also shows incidentally how $\mathscr{E}(\rho, z)$ can be deduced uniquely in terms of $\mathscr{E}(0, z)$ from the HHP.

Finally, in order to explicitly calculate $h(t)$ for any given solution $\mathscr{E}$, one need only introduce the flat space expression in the right-hand side of Eq. (A15). For flat space,[9]

$$F(t) = \begin{pmatrix} \dfrac{t}{S(t)} & \dfrac{i}{S(t)} \\ -\dfrac{it\nu(t)}{S(t)} & \dfrac{\mu(t)}{S(t)} \end{pmatrix}, \tag{A20}$$

where

$$\mu(t) = \frac{1 - 2tz - S(t)}{2t}, \quad \nu(t) = \frac{1 - 2tz + S(t)}{2t}. \tag{A21}$$

It follows that $h(t)$ for flat space is given by

$$h(t) = \begin{pmatrix} 0 & -t^{-1} \\ t & 0 \end{pmatrix}. \tag{A22}$$

Hence, substituting Eqs. (A19) and (A22) into Eq. (A15), we find that $h(t)$ for any solution $\mathscr{E} = f + i\psi$ in special HE gauge is given by

$$h(t) = \begin{pmatrix} -\psi f^{-1} & -t^{-1}f^{-1} \\ t(f + \psi^2 f^{-1}) & \psi f^{-1} \end{pmatrix}, \tag{A23}$$

with f and ψ evaluated at $\rho = 0, z = (2t)^{-1}$. Notice that the HE boundary condition that

$$F(t)\begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix}$$

be analytic at $t = \infty$ is satisfied on both Riemann sheets. Notice also that if $h(t)$ is known, then $\mathscr{E}(0, z)$ can be deduced immediately from Eq. (A23), and then $\mathscr{E}(\rho, z)$ and $F(t)$ are determined uniquely by the HHP.

Although the $F(t)$ potential for the general Weyl solution, $\mathscr{E} = e^{2\chi}$, $\chi_{\rho\rho} + \rho^{-1}\chi_\rho + \chi_{zz} = 0$, is well known, it is not at all obvious how to identify which gauge is special HE gauge. The expression given in Ref. 12 can be written

$$F(t) = \begin{pmatrix} e^{\chi} & 0 \\ 0 & e^{-\chi} \end{pmatrix}\begin{pmatrix} \dfrac{t}{S(t)} & \dfrac{i}{S(t)} \\ -\dfrac{it\nu(t)}{S(t)} & \dfrac{\mu(t)}{S(t)} \end{pmatrix}\begin{pmatrix} e^{\beta(t)} & 0 \\ 0 & e^{-\beta(t)} \end{pmatrix}, \tag{A24}$$

where $\beta(t) = \beta(\rho, z, t)$ satisfies

$$\nabla\beta(t) = \frac{(1 - 2tz)\nabla\chi - 2t\rho\tilde{\nabla}\chi}{S(t)}, \quad \beta(0) = \chi. \tag{A25}$$

$\beta(t)$ is defined up to an arbitrary additive function of t only. This arbitrariness corresponds to the freedom to change gauge in $F(t)$ with a diagonal $g(t)$ matrix. Since $\nabla\beta(t)$ is odd in $S(t)$, there is a natural particular integral of Eq. (A25), which we denote $\beta_{\text{odd}}(t)$, which is also odd in $S(t)$. This natural gauge for the Weyl $F(t)$-potential is precisely the gauge used by KC to derive the Kerr and generalized Tomimatsu–Sato solutions from special Weyl solutions.[10] In Ref. 16, we calculated $\tilde{F}(t)$ with the choice $\beta(t) = \beta_{\text{odd}}(t)$ and found that $h(t)$ is the same for all Weyl solutions and is given by the flat space expression (A22). However, this natural gauge is *not* special HE gauge (except for flat space) as $\beta_{\text{odd}}(t)$ has (ρ, z)-independent singularities in the complex t plane. A direct calculation shows that if

$$\beta(t) = \beta_{\text{odd}}(t) + \delta(t) \tag{A26}$$

in Eq. (A24), where $\delta(t)$ is some function of t only, then

$$h(t) = \begin{pmatrix} 0 & -t^{-1}e^{-2\delta(t)} \\ te^{2\delta(t)} & 0 \end{pmatrix}. \tag{A27}$$

If $F(t)$ is in special HE gauge, then $e^{\pm\beta(t)}$ must be analytic throughout the t plane (including $t = \infty$) except for quadratic branch points at the zeros of $S(t)$. In that case, $\delta(t)$ is uniquely determined by equating the right-hand sides of Eqs. (A27) and (A23) with $f = e^{2\chi}$, $\psi = 0$. The result is

$$\delta(t) = \chi(0, (2t)^{-1}). \tag{A28}$$

A direct proof of this result can be obtained from the contour integral expression (3.47b) by observing that the residue of the integrand at $t' = t$ is even in $S(t)$ and the remainder of the integral is odd in $S(t)$ and that $\xi(t) = -\chi(0, (2t)^{-1})$.

APPENDIX B: RELATIONSHIP BETWEEN $\psi(\lambda)$ AND $\psi(\alpha^2/\lambda)$

The complex spectral parameter λ used by Belinskii and Zakharov[2] (BZ) is related to t by the quadratic transformation,[16]

$$t = t(\lambda) = \lambda/(\lambda^2 + 2\beta\lambda + \alpha^2), \tag{B1}$$

so that the image of the full λ plane is the two-sheeted Riemann t surface which is the domain of $S(t)$ with branch points at the two zeros,

$$t = \tfrac{1}{2}(\beta \pm \alpha)^{-1}, \tag{B2}$$

of $S(t)$. To fix ideas, we consider (α, β) domains for which $|\beta| > \alpha > 0$. Then the branch cut may be taken as the finite segment of the real axis joining the zeros and not passing through $t=0$. For t on the first Riemann sheet (excluding cut, including $t=\infty$), the inverse of Eq. (B1) is

$$\lambda=\mu(t)=[1-2t\beta-S(t)]/2t, \tag{B3a}$$

and the image in the λ plane is the open disk, $|\lambda|<\alpha$, denoted Γ_2 (note $t=0$ implies $\lambda=0$). For t on the second Riemann sheet (excluding cut, including $t=\infty$), the inverse of Eq. (B1) is

$$\lambda=\nu(t)=[1-2t\beta+S(t)]/2t=\alpha^2/\mu(t), \tag{B3b}$$

and the image in the λ plane is the region, $|\lambda|>\alpha$, denoted Γ_1, as well as $\lambda=\infty$. The two zeros of $\lambda^2+2\beta\lambda+\alpha^2$, namely $\lambda=\lambda_2$ in Γ_2 and $\lambda=\lambda_1$ in Γ_1, map to the two points at infinity of the Riemann t surface. The circle $|\lambda|=\alpha$ (denoted Γ) maps one-to-two onto the branch cut itself. To understand this a little better, consider counterclockwise circles, $|\lambda|=\alpha-\delta$ in Γ_2 and $|\lambda|=\alpha+\delta$ in Γ_1, where δ is small and positive. The former maps to a clockwise closed curve enclosing and closely fitting the cut in the t plane, the latter to a similar but counterclockwise curve on the second Riemann sheet.

The BZ matrix eigenfunction $\psi(\lambda)$ is related to $F(t)$ by[16]

$$\psi(\lambda)=t^{-1}S(t)P(t),\quad |\lambda|<\alpha, \tag{B4}$$

where the matrix functions $P(t)$ and $Q(t)$ are defined by

$$F(t)=P(t)+iQ(t),\quad F^*(t)=P(t)-iQ(t). \tag{B5}$$

This result was proved in Ref. 16 by directly comparing the differential equations for $\psi(\lambda)$ and $P(t)$. The differential equations also allow a multiplicative matrix function of t only (reducing to the unit matrix at $t=0$) on the right of Eq. (B4) (gauge change + t-dependent rescaling) but without loss of generality we set it to be identically unity in order that $\psi(\lambda)$ be analytic in Γ_2 whenever $F(t)$ is in special HE gauge. The HE condition (1.11) at $t=\infty$ also implies corresponding conditions on $\psi(\lambda)$ at the two zeros of $\lambda^2+2\beta\lambda+\alpha^2$ [see Eq. (2.4)].

Analytic continuation of Eq. (B4) to $|\lambda|>\alpha$ gives, with an obvious notation,

$$\psi(\lambda)=-t^{-1}S(t)\tilde{P}(t),\quad |\lambda|>\alpha, \tag{B6a}$$

or, equivalently,

$$\psi(\alpha^2/\lambda)=-t^{-1}S(t)\tilde{P}(t),\quad |\lambda|<\alpha. \tag{B6b}$$

[In Eq. (B6a), $\lambda=\nu(t)$; in Eq. (B6b), $\lambda=\mu(t)$, $\alpha^2/\lambda=\nu(t)$.] Now, from Eqs. (B5) and (A11),

$$\tilde{P}(t)=-Q(t)h(t),\quad \tilde{Q}(t)=P(t)h(t), \tag{B7a,b}$$

where $h(t)$ is given by Eq. (A23) if $F(t)$ is in special HE gauge, and from Eqs. (A16a,b) otherwise. We reproduce here some simple identities given in Ref. 16 which are immediate consequences of Eqs. (A7a,b) here:

$$P(t)=-\nu^{-1}(t)\mathbf{g}\boldsymbol{\epsilon}Q(t),\quad Q(t)=\mu^{-1}(t)\mathbf{g}\boldsymbol{\epsilon}P(t), \tag{B8a,b}$$

$$\det P(t)=t\mu(t)/S^2(t),\quad \det Q(t)=t\nu(t)/S^2(t), \tag{B9a,b}$$

$$\det\psi(\lambda)=\lambda^2+2\beta\lambda+\alpha^2. \tag{B10}$$

From Eqs. (B7a) and (B8b), we have

$$\tilde{P}(t)=-\mu^{-1}(t)\mathbf{g}\boldsymbol{\epsilon}P(t)h(t). \tag{B11}$$

Finally, from Eqs. (B4) and (B6b), we obtain the desired relationship:

$$\psi(\alpha^2/\lambda)=\lambda^{-1}\mathbf{g}\boldsymbol{\epsilon}\psi(\lambda)h(t). \tag{B12}$$

Although Eq. (B12) was derived for $|\lambda|<\alpha$, it holds for all λ. This can be seen from the inverse relation

$$\begin{aligned}\psi(\lambda)&=-\lambda\boldsymbol{\epsilon}\mathbf{g}^{-1}\psi(\alpha^2/\lambda)h(t)^{-1}\\&=(\lambda/\alpha^2)\mathbf{g}\boldsymbol{\epsilon}\psi(\alpha^2/\lambda)h(t),\end{aligned} \tag{B13}$$

where we have used $\boldsymbol{\epsilon}^{-1}=-\boldsymbol{\epsilon}$, $\det\mathbf{g}=\alpha^2$, $h(t)^{-}=-h(t)$, the symmetry of $\mathbf{g}$, and the following identity satisfied by any nondegenerate matrix M:

$$\boldsymbol{\epsilon}M^T\boldsymbol{\epsilon}=-(\det M)M^{-1}, \tag{B14}$$

^{T} denoting matrix transpose.

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[30] Condition (1.11) requires that $\omega = 0$ [see Eq. (1.4)] on the z axis near (0,0). If $\omega(0,0) \neq 0$, then the theorem holds except that condition (1.11) should be replaced by the weaker condition that $F(t)$ only be analytic at $t = \infty$, and the gauge is unique up to one arbitrary constant. This slightly more general gauge is called "modified special HE gauge" in Ref. 11. Equation (A2) and the analyticity of $\mathscr{E}(\rho,z)$ imply that $\omega(0,z)$ is constant, say b, and so condition (1.11) can be brought about by a coordinate transformation, $x'^1 = x^1 - bx^2$, $x'^2 = x^2$, in the metric (1.1) or (1.3). The effect on the $F(t)$ potential is given by

$$F'(t) = \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix} F(t) \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix},$$

and the representing matrix is

$$u(t) = \begin{pmatrix} 1 & -b \\ 0 & 1 \end{pmatrix}.$$

When modified special HE gauge is under consideration, condition (1.13d) on $u(t)$ should be replaced by analyticity of $u(t)$ at $t = \infty$.
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[39] Equations (7.16) and (7.17) of Ref. 16 give the transforms of $G_{AB}(t_1,t_2)$ and $F_{AB}(t)$, respectively, under the $s = \infty$ nonnull HKX transformation. Due to a printing error, the first part of Eq. (7.16) was omitted. The omitted part should read

$$G'_{AB}(t_1,t_2) = G_{AB}(t_1,t_2) + \cdots .$$

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Consistency of the Cauchy initial value problem in a nonsymmetric theory of gravitation

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The consistency of the Cauchy initial value problem in a theory of gravity based on a nonsymmetric metric is investigated. It is demonstrated that the dynamical equations preserve the constraint equations as the evolution of the initial data occurs. The consistency is shown rigorously using the full field equations rather than the series expansion used previously.

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I. INTRODUCTION

A new theory of gravitation has recently been proposed and developed.[1-3] The theory is based on a nonsymmetric metric $g_{\mu\nu}$ and the two premises:

(i) The transposition-invariant (Hermitian) length of a vector, A^μ, given by $(g_{\mu\nu}A^\mu \overline{A^\nu})$, is preserved under parallel transport with respect to a connection $A^\lambda_{\mu\nu}(\Gamma^\lambda_{\mu\nu}$ in free space);

(ii) A local inertial frame of reference exists such that at a point $x^\mu = x'^\mu$,

$$A^\lambda_{(\mu\nu)}|_{x=x'} = 0.$$

The theory has been shown to possess a rigorous spherically symmetric solution of the vacuum equations.[1] When the known solutions of the theory are analyzed, radical departures from general relativity are seen at small distances (static solutions)[1] and early times (cosmological solutions).[4,5] The theory agrees with all current relativity experiments.[1,6]

The formalism for the Cauchy problem has been previously set up[7] by considering an expansion of the metric $g_{\mu\nu}$ about Minkowski space, $\eta_{\mu\nu}$. This is necessary at present, because of the difficulty in working with the closed form of the metric connection $\Gamma^\lambda_{\mu\nu}$.[8] This paper is concerned with the consistency of what appears to be an overdetermined system of equations for the forward propagation of $g_{\mu\nu}$, in time, thus completing the work mentioned in Ref. 7.

II. FIELD EQUATIONS AND IDENTITIES

The vacuum field equations can be derived by a Palatini variation from the vacuum Lagrangian density[1,7]

$$L = \mathbf{g}^{\mu\nu}R_{\mu\nu}(W), \tag{2.1}$$

where we have used the notation $\mathbf{X} = (\sqrt{-g})X$ and

$$R_{\mu\nu}(W) = W^\beta_{\mu\nu,\beta} - \tfrac{1}{2}(W^\beta_{\mu\beta,\nu} + W^\beta_{\nu\beta,\mu}) - W^\beta_{\alpha\nu}W^\alpha_{\mu\beta} + W^\beta_{\alpha\beta}W^\alpha_{\mu\nu}. \tag{2.2}$$

Here $W^\lambda_{\mu\nu}$ is a nonsymmetric affine connection. Performing the variation yields the field equations

$$g_{\mu\nu,\sigma} - g_{\rho\nu}\Gamma^\rho_{\mu\sigma} - g_{\mu\rho}\Gamma^\rho_{\sigma\nu} = 0, \tag{2.3}$$

$$\mathbf{g}^{[\mu\nu]}{}_{,\nu} = 0, \tag{2.4}$$

$$R_{\mu\nu}(\Gamma) = \tfrac{2}{3}W_{[\nu,\mu]}, \tag{2.5}$$

where $\Gamma^\lambda_{\mu\nu}$ is a Hermitian connection related to $W^\lambda_{\mu\nu}$ by

$$W^\lambda_{\mu\nu} = \Gamma^\lambda_{\mu\nu} - \tfrac{2}{3}\delta^\lambda_\mu W_\nu \tag{2.6}$$

and W_ν is given by

$$W_\nu = W^\lambda_{[\nu\lambda]} = \tfrac{1}{2}(W^\lambda_{\nu\lambda} - W^\lambda_{\lambda\nu}). \tag{2.7}$$

Equation (2.6) guarantees the four conditions $\Gamma_\mu = \Gamma^\lambda_{[\mu\lambda]} = 0$, which are equivalent to the four equations (2.4). The contracted curvature tensor $R_{\mu\nu}(\Gamma)$ is

$$R_{\mu\nu}(\Gamma) = \Gamma^\beta_{\mu\nu,\beta} - \tfrac{1}{2}(\Gamma^\beta_{(\mu\beta),\nu} + \Gamma^\beta_{(\nu\beta),\mu}) - \Gamma^\beta_{\alpha\nu}\Gamma^\alpha_{\mu\beta} + \Gamma^\beta_{(\alpha\beta)}\Gamma^\alpha_{\mu\nu}. \tag{2.8}$$

W_μ represents an auxiliary vector field and the Lagrangian (2.1) is invariant under the abelian gauge transformation[1]

$$W'_\mu = W_\mu + \lambda_{,\mu}, \tag{2.9}$$

where λ is an arbitrary scalar field.

The coordinate and gauge invariance of the Lagrangian can be used to generate five identities of the theory.[9] Four of these are generalized Bianchi identities:

$$[\mathbf{g}^{\alpha\nu}G_{\rho\nu}(\Gamma) + \mathbf{g}^{\nu\alpha}G_{\nu\rho}(\Gamma)]_{,\alpha} + g^{\mu\nu}{}_{,\rho}\mathbf{G}_{\mu\nu}(\Gamma) = 0, \tag{2.10}$$

where

$$G_{\rho\nu}(\Gamma) = R_{\rho\nu}(\Gamma) - \tfrac{1}{2}g_{\rho\nu}R(\Gamma) \tag{2.11}$$

with

$$R(\Gamma) = g^{\alpha\beta}R_{\alpha\beta}(\Gamma). \tag{2.12}$$

The remaining identity can be written as

$$\mathbf{g}^{[\mu\nu]}{}_{,\nu,\mu} = 0. \tag{2.13}$$

III. THE CAUCHY PROBLEM

Consider a three dimensional hypersurface S oriented in space. We can choose, without loss of generality, a coordinate system such that the surface S is described by $x^0 = 0$. On S we are given the initial data $g_{(\mu\nu)}, g_{(\mu\nu),0}, g_{[ij]}, g_{[ij],0}, g_{[0i]}$, and W_i with the restriction $g_{00} > 0$. We can then calculate all the interior derivatives of $g_{\mu\nu}$ and W_i on S. The gauge freedom of W_μ [Eq. (2.9)] can be used to set $W_0 = 0$.

It has been shown by Moffat[7] that under a flat space expansion of $g_{\mu\nu}$, the nth order field equations can be rewritten as a set of dynamical equations ($i, j = 1, 2, 3$):

$$\overset{(n)}{g}_{(ij),00} = 2\overset{(n)}{N}_{(ij)} + 2\overset{(n)}{K}_{(ij)}, \tag{3.1}$$

$$\overset{(n)}{g}_{[ij],00} = \nabla^2 \overset{(n)}{g}_{[ij]} + \overset{(n)}{K}_{[ij]} + \tfrac{1}{3}\overset{(n)}{W}_{[i,j]}, \tag{3.2}$$

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$$\overset{(n)}{W}_{i,0} = \tfrac{3}{4}\overset{(n)}{g}_{[ij],0j} - \tfrac{3}{4}\nabla^2 \overset{(n)}{g}_{[i0]} + \overset{(n)}{L}_{[i0]}, \tag{3.3}$$

$$\overset{(n)}{g}_{[i0],00} = \overset{(n)}{g}_{[ij],0j} + \overset{(n)}{C}_{[i,0]}, \tag{3.4}$$

where the right-hand sides are determined by the initial data, interior derivatives, and the lower order dynamical equations. As well, there is an additional set of constraint equations:

$$\overset{(n)}{R}_{(i0)} = 0, \tag{3.5}$$

$$\overset{(n)}{R}_{00} = 0, \tag{3.6}$$

$$\overset{(n)}{\mathbf{g}}{}^{[0i]}{}_{,i} = 0, \tag{3.7}$$

which can be rewritten in the form of initial data constraints. The compatibility of the above systems has been demonstrated by Moffat.[7]

The nature of the dynamical equations is such that they can be integrated forward in time consistently, provided the constraint equations remain true once they are fulfilled at $x^0 = 0$.

IV. CONSISTENCY

The dynamical set of equations is derived from the field equations $(i,j = 1,2,3)$

$$R_{(ij)} = 0, \tag{4.1}$$

$$R_{[\mu\nu]} = \tfrac{2}{3} W_{[\nu,\mu]}, \tag{4.2}$$

$$\mathbf{g}^{[i\mu]}{}_{,\mu} = 0, \tag{4.3}$$

and the initial constraint set of equations is derived from

$$R_{(i0)} = 0, \tag{4.4}$$

$$R_{00} = 0, \tag{4.5}$$

$$\mathbf{g}^{[0i]}{}_{,i} = 0. \tag{4.6}$$

The equations to be investigated are (4.4)–(4.6). The objective is to show that the existence of the dynamical equations (4.1)–(4.3) is sufficient to maintain the validity of the constraint equations (4.4)–(4.6) for all x^0, once the constraint equations are satisfied at $x^0 = 0$.

If we rewrite (4.3) as

$$\mathbf{g}^{[i0]}{}_{,0} + \mathbf{g}^{[ij]}{}_{,j} = 0 \tag{4.7}$$

and take the divergence, we find

$$\mathbf{g}^{[i0]}{}_{,i0} = 0. \tag{4.8}$$

When this is combined with the initial constraint

$$\mathbf{g}^{[i0]}{}_{,i} = 0 \quad \text{at} \quad x^0 = 0, \tag{4.9}$$

we have the unique solution of (4.8),

$$\mathbf{g}^{[i0]}{}_{,i} = 0 \quad \text{for all} \quad x^0. \tag{4.10}$$

Thus Eq. (4.6) is maintained for all x^0.

Now consider the Bianchi identities (2.10). If we substitute for $G_{\mu\nu}(\Gamma)$ and $R(\Gamma)$ with (2.11)–(2.12) and utilize the relationship

$$g^{\mu\nu}{}_{,\rho}\mathbf{g}_{\mu\nu} = -2(\sqrt{-g})_{,\rho}, \tag{4.11}$$

we find after some algebra

$$[\mathbf{g}^{\alpha\nu}R_{\rho\nu} + \mathbf{g}^{\nu\alpha}R_{\nu\rho}]_{,\alpha} - \mathbf{g}^{\mu\nu}R_{\mu\nu,\rho} = 0. \tag{4.12}$$

Separating $g^{\alpha\beta}$ and $R_{\alpha\beta}$ into symmetric and skew parts, Eq. (4.12) becomes

$$R_{(\rho\nu)}\mathbf{g}^{(\alpha\nu)}{}_{,\alpha} + \mathbf{g}^{(\alpha\nu)}R_{(\rho\nu),\alpha} + R_{[\rho\nu]}\mathbf{g}^{[\alpha\nu]}{}_{,\alpha} + \tfrac{1}{2}\mathbf{g}^{[\alpha\nu]}R_{[\rho\nu,\alpha]} - \tfrac{1}{2}\mathbf{g}^{(\mu\nu)}R_{(\mu\nu),\rho} = 0 \tag{4.13}$$

with

$$R_{[\rho\nu,\alpha]} = R_{[\rho\nu],\alpha} + R_{[\nu\alpha],\rho} + R_{[\alpha\rho],\nu}. \tag{4.14}$$

That $R_{[\rho\nu,\alpha]} = 0$ can be seen immediately by considering Eq. (4.2), which is valid for all x^0 because it is part of the dynamical system of equations. Also the term $\mathbf{g}^{[\alpha\nu]}{}_{,\alpha}R_{[\rho\nu]}$ can be seen to be zero by writing it as

$$\mathbf{g}^{[\alpha\nu]}{}_{,\alpha}R_{[\rho\nu]} = \mathbf{g}^{[\alpha0]}{}_{,\alpha}R_{[\rho0]} + \mathbf{g}^{[\alpha i]}{}_{,\alpha}R_{[\rho i]}, \tag{4.15}$$

where $\mathbf{g}^{[\alpha0]}{}_{,\alpha} = 0$ by Eq. (4.10) and $\mathbf{g}^{[\alpha i]}{}_{,\alpha} = 0$ by Eq. (4.3). Thus Eq. (4.13) becomes

$$R_{(\rho\nu)}\mathbf{g}^{(\alpha\nu)}{}_{,\alpha} + \mathbf{g}^{(\alpha\nu)}R_{(\rho\nu),\alpha} - \tfrac{1}{2}\mathbf{g}^{(\mu\nu)}R_{(\mu\nu),\rho} = 0. \tag{4.16}$$

We now rewrite Eq. (4.16) as two sets of equations by considering $\rho = 0$ and k $(k = 1,2,3)$,

$$R_{(0\nu)}\mathbf{g}^{(\alpha\nu)}{}_{,\alpha} + \mathbf{g}^{(\alpha\nu)}R_{(0\nu),\alpha} - \tfrac{1}{2}\mathbf{g}^{(\mu\nu)}R_{(\mu\nu),0} = 0, \tag{4.17a}$$

$$R_{(k\nu)}\mathbf{g}^{(\alpha\nu)}{}_{,\alpha} + \mathbf{g}^{(\alpha\nu)}R_{(k\nu),\alpha} - \tfrac{1}{2}\mathbf{g}^{(\mu\nu)}R_{(\mu\nu),k} = 0. \tag{4.17b}$$

From Eq. (4.1) we have $R_{(ij)} = 0$ identically for all x^μ; thus all derivatives of $R_{(ij)}$ vanish and we have

$$R_{(ij),\mu} = 0. \tag{4.18}$$

Expanding the terms in Eqs. (4.17a) and (4.17b) by separating the summed indices into space and time parts and using Eqs. (4.1) and (4.18) we have

$$R_{00,0} = \frac{-2}{\mathbf{g}^{00}}\{R_{(0\nu)}\mathbf{g}^{(\alpha\nu)}{}_{,\alpha} + \mathbf{g}^{(j\nu)}R_{(0\nu),j}\}, \tag{4.19a}$$

$$R_{(0k),0} = -\frac{1}{\mathbf{g}^{00}}\{R_{(0k)}\mathbf{g}^{(\alpha0)}{}_{,0} + \mathbf{g}^{(0j)}R_{(0k),j} - \tfrac{1}{2}\mathbf{g}^{00}R_{00,k} - \mathbf{g}^{(0j)}R_{(0j),k}\}. \tag{4.19b}$$

The left-hand sides of (4.19a) and (4.19b) contain all the time developments of R_{00} and $R_{(0k)}$ while the right-hand sides depend only on the metric tensor, its derivatives, and the interior derivatives of of R_{00} and $R_{(0k)}$. If we assume the analytic behavior of the metric tensor, then this system has a unique solution when combined with the initial constraints

$$R_{00} = 0, \quad R_{(0k)} = 0 \quad \text{at} \quad x^0 = 0.$$

The solution is

$$R_{00} = 0, \quad R_{(0k)} = 0 \quad \text{for all } x^0.$$

Thus Eqs. (4.4) and (4.5) are maintained once they are satisfied on the initial hypersurface S.

V. CONCLUSION

We have demonstrated that the constraint equations are maintained by the dynamical system, thus making it possible to consistently integrate the metric and W_μ field forward in time from the original hypersurface S. In the work presented, we have shown this result in a manner dependent only on the analytic behavior of the metric and not on the flat space expansion, thereby making the consistency rigorous.

This work, when combined with that of Ref. 7, leads to a solution of the Cauchy problem within the context of the new gravitation theory,[1] provided the flat space expansions in Ref. 7 converge. There still remains the problem of finding a rigorous dynamical solution for the $g_{\mu\nu}$ using a closed form for the $\Gamma^{\lambda}_{\mu\nu}$.

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Kerr-like metric in Brans–Dicke theory

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A Kerr-like metric is obtained by means of a complex coordinate transformation in the Brans–Dicke theory.

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Newman and Janis[1] have given a derivation of the Kerr metric by performing a complex coordinate transformation on the Schwarzschild metric. Later, Newman *et al.*[2] applied a similar technique to the Reissner–Nordstrom solution to obtain the charged Kerr metric (Kerr–Newman solution). In this paper we have followed a similar procedure to obtain the metric of a rotating body in the Brans–Dicke theory. Coordinate transformations have been made on the usual Brans–Dicke metric[3] to bring the line element formally into the standard Schwarzschild-like form. Then, complex coordinate transformations have been carried out and the Kerr-like metric is obtained in the Brans–Dicke theory.

The Brans–Dicke line element in isotropic form[3] may be written as

$$ds^2 = e^{2\alpha_0}\left[\frac{1-B/r}{1+B/r}\right]^{2/\lambda} dt^2 - e^{2\beta_0}(1+B/r)^4 \times \left[\frac{1-B/r}{1+B/r}\right]^{2(\lambda-c-1)/\lambda}[dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2)]. \quad (1)$$

By making a change of scale $r \to re^{\beta_0}$, $t \to te^{\alpha_0}$ of the coordinates r and t, the line element (1) becomes

$$ds^2 = \left(\frac{1-r_0/r}{1+r_0/r}\right)^{2/\lambda} dt^2 - (1+r_0/r)^4\left[\frac{1-r_0/r}{1+r_0/r}\right]^{2(\lambda-c-1)/\lambda} \times [dr^2 + r^2(d\theta^2 + \sin\theta\, d\phi^2)], \quad (2)$$

where $r_0 = Be^{\beta_0}$. Substituting $\bar r$ in place of r with the help of the relation

$$\bar r = r(1+\bar r_0/2r)^2, \quad (3)$$

in Eq. (2), we have

$$ds^2 = (1-2\bar r_0/\bar r)^{\eta} dt^2 - (1-2\bar r_0/\bar r)^{\xi-1} d\bar r^2 - \bar r^2(1-2\bar r_0/\bar r)^{\xi} d\theta^2 - \bar r^2(1-2\bar r_0/\bar r)^{\xi}\sin^2\theta\, d\phi^2, \quad (4)$$

where

$$\eta = 1/\lambda,\ \xi = (\lambda - c - 1)/\lambda, \text{ and } \bar r_0 = 2r_0. \quad (5)$$

We now choose a time coordinate u such that

$$du = dt - (1-2\bar r_0/\bar r)^{(\xi-\eta-1)/2} d\bar r. \quad (6)$$

With the help of (6) the line element (4) becomes,

$$ds^2 = (1-2\bar r_0/\bar r)^{\eta} du^2 + 2(1-2\bar r_0/\bar r)^{(\eta+\xi-1)/2} du\,dr \times - \bar r^2(1-2\bar r_0/\bar r)^{\xi} d\theta^2 - \bar r^2(1-2\bar r_0/\bar r)^{\xi}\sin^2\theta\, d\phi^2. \quad (7)$$

The contravariant components of metric (7)

$$g^{44} = 0,$$
$$g^{11} = -(1-2\bar r_0/\bar r)^{1-\xi},$$
$$g^{14} = (1-2\bar r_0/\bar r)^{-(\eta+\xi-1)/2},$$
$$g^{22} = (-1/\bar r^2)(1-2\bar r_0/\bar r)^{-\xi},$$
$$g^{33} = (-1/\bar r^2\sin^2\theta)(1-2\bar r_0/\bar r)^{-\xi},$$

can be represented in the alternate form

$$g^{\mu\nu} = l^\mu n^\nu + l^\nu n^\mu - m^\mu \bar m^\nu - m^\nu \bar m^\mu, \quad (8)$$

where

$$l^\mu = \delta^\mu_1,\quad n^\mu = [1-2\bar r_0/\bar r]^{-(\eta+\xi-1)/2}\delta^\mu_4 - \tfrac{1}{2}[1-2\bar r_0/\bar r]^{1-\xi}\delta^\mu_1,$$
$$m^\mu = \left[\sqrt{2}\bar r(1-2\bar r_0/\bar r)^{\xi/2}\right]^{-1}[\delta^\mu_2 + (i/\sin\theta)\delta^\mu_3], \quad (9)$$
$$\bar m^\mu = \left[\sqrt{2}\bar r(1-2\bar r_0/\bar r)^{\xi/2}\right]^{-1}[\delta^\mu_2 - (i/\sin\theta)\delta^\mu_3].$$

(The previous use of bars on r is dropped and any bar now appearing on r indicates its complex conjugate value.)

The coordinate r is allowed to take complex values and the tetrad is rewritten in the form

$$l^\mu = \delta^\mu_1,\quad n^\mu = [1 - r_0(1/r + 1/\bar r)]^{-(\eta+\xi-1)/2}\delta^\mu_4 - \tfrac{1}{2}[\{1 - r_0(1/r+1/\bar r)\}]^{1-\xi}\delta^\mu_1,$$
$$m^\mu = \left[\sqrt{2}r\{1 - r_0(1/r+1/\bar r)\}^{\xi/2}\right]^{-1}[\delta^\mu_2 + (i/\sin\theta)\delta^\mu_3], \quad (10)$$
$$\bar m^\mu = \left[\sqrt{2}r\{1 - r_0(1/r+1/\bar r)\}^{\xi/2}\right]^{-1}[\delta^\mu_2 - (i/\sin\theta)\delta^\mu_3].$$

(l^μ and n^μ are kept real and m^μ and $\bar m^\mu$ the complex conjugates of each other.)

We now formally perform the complex coordinate transformation

$$r' = r + ia\cos\theta,\quad \theta' = \theta, \qquad u' = u - ia\cos\theta,\quad \phi' = \phi, \quad (11)$$

on vectors l^μ, n^μ and m^μ($\bar m'^\mu$ is defined as the complex conjugate of m'^μ).

If one allows r' and u' to be real, we define the following tetrad

$$l'^\mu = \delta^\mu_1,\quad n'^\mu = \left[1 - \frac{2r_0 r'}{r'^2 + a^2\cos^2\theta}\right]^{-(\eta+\xi-1)/2}\delta^\mu_4 - \tfrac{1}{2}\left[1 - \frac{2r_0 r'}{r'^2 + a^2\cos^2\theta}\right]^{1-\xi}\delta^\mu_1$$

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$$m'^{\mu} = \left[\sqrt{2}(r' + ia\cos\theta)\left(1 - \frac{2r_0 r'}{r'^2 + a^2\cos^2\theta}\right)^{\xi/2}\right]^{-1}$$
$$\times [ia\sin\theta\,(\delta_4^{\mu} - \delta_1^{\mu}) + \delta_2^{\mu} + (i/\sin\theta)\delta_3^{\mu}],$$
$$\bar{m}'^{\mu} = \left[\sqrt{2}(r' - ia\cos\theta)\left(1 - \frac{2r_0 r'}{r'^2 + a^2\cos^2\theta}\right)^{\xi/2}\right]^{-1}$$
$$\times [-ia\sin\theta\,(\delta_4^{\mu} - \delta_1^{\mu}) + \delta_2^{\mu} - (i/\sin\theta)\delta_3^{\mu}]. \qquad (12)$$

The metric coefficient $g^{\mu\nu}$ now takes the form

$$g'^{\mu\nu} = l'^{\mu}n'^{\nu} + l'^{\nu}n'^{\mu} - m'^{\mu}\bar{m}'^{\nu} - m'^{\nu}\bar{m}'^{\mu}. \qquad (13)$$

From (12) and (13) the desired line element may be written as (dropping the prime)

$$ds^2 = \left[1 - \frac{2r_0 r}{r^2 + a^2\cos^2\theta}\right]^{\eta}(du - a\sin^2\theta\, d\phi)^2$$
$$+ 2\left[1 - \frac{2r_0 r}{r^2 + a^2\cos^2\theta}\right]^{(\eta+\xi-1)/2}$$
$$\times (du - a\sin^2\theta\, d\phi)(dr + a\sin^2\theta\, d\phi)$$
$$- \left[1 - \frac{2r_0 r}{r^2 + a^2\cos^2\theta}\right]^{\xi}(r^2 + a^2\cos^2\theta)$$
$$\times (d\theta^2 + \sin^2\theta\, d\phi^2). \qquad (14)$$

Metric (14) represents the axially symmetric gravitational field of a rotating mass in Brans–Dicke theory. There is no dependence of the line element on the angular coordinate ϕ so that the solution (14) is manifestly axially symmetric.

A further simplification is made by another coordinate transformation so as to make the line element (14) as similar as possible to that of rotating flat space which contains only one off-diagonal term in the metric tensor, a term in $d\phi dt$.

The desired transformation is[4]

$$du = d\hat{t} + A dr, \quad d\phi = d\hat{\phi} + B dr, \qquad (15)$$

where A and B are functions of r only. The values of A and B are

$$A = -\frac{[a^2\sin^2\theta + (r^2 + a^2\cos^2\theta)(1 - 2r_0 r/(r^2 + a^2\cos^2\theta))^{(\xi-\eta+1)/2}]}{r^2 + a^2 - 2r_0 r},$$
$$B = \frac{-a(1 - 2r_0 r/(r^2 + a^2\cos^2\theta))^{-(\eta+\xi-1)/2}}{r^2 + a^2 - 2r_0 r}.$$

Then, the coefficient of dr^2 is

$$-\frac{r^2 + a^2\cos^2\theta}{r^2 + a^2 - 2r_0 r}\left(1 - \frac{2r_0 r}{r^2 + a^2\cos^2\theta}\right)^{\xi}.$$

In view of (15), the metric (14) (dropping the carets on t and ϕ), may be written as

$$ds^2 = (1 - 2r_0 r/\rho)^{\eta}(dt - \omega\, d\phi)^2$$
$$- (1 - 2r_0 r/\rho)^{\xi}\rho(dr^2/\Delta + d\theta^2 + \sin^2\theta\, d\phi^2)$$
$$+ 2(1 - 2r_0 r/\rho)^{\sigma}\omega(dt - \omega\, d\phi)d\phi, \qquad (16)$$

where

$\omega = a\sin^2\theta$, $\rho = r^2 + a^2\cos^2\theta$, $\Delta = r^2 + a^2 - 2r_0 r$, and $\sigma = (n + \xi - 1)/2 = -c/2\lambda$.

The expression for Φ (Brans–Dicke scalar field) is

$$\Phi = \Phi_0(1 - 2r_0 r/\rho)^{\sigma}, \qquad (17)$$

where Φ_0 is a constant.

A check has been made on the Brans–Dicke field equations and it has been found that (16) and (17) satisfy them.

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On the structure of the generalized Tjon–Wu equations

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The kinetic equations proposed by Ziff are analyzed and their connection with the homogeneous Boltzmann equation is discussed. For a family of models generalizing the Tjon–Wu and Bobylev–Krook–Wu equations, the ordinary and Laguerre moment equations are considered. Beyond the existence of a unique solution in L^1, conditions for the convergence of the Laguerre expansion are found and asymptotic estimates are given.

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INTRODUCTION

The Tjon–Wu (T.W.) equation[1] is the prototype of a class of kinetic equations describing the time evolution of a spatially homogeneous system of identical particles whose collisions conserve energy and may or may not conserve momentum. The general structure of such equations first proposed by Futcher *et al.*[2] was discussed by Ziff[3] and the connection with the *d*-dimensional Boltzmann equation (B.E.) was given for special models by Ernst and Hendriks.[4] Barnsley and Turchetti investigated the connection with the 3-dimensional B.E. for arbitrary cross section.[5] The same authors proved that a B.E. for Maxwell-like molecules, for which Bobylev, Krook, and Wu (B.K.W.) provided an explicit solution,[6,7] was related to the T. W. equation by an Abel transformation.[8] The method of integral transforms allowed the construction of new models,[4] all solvable via a Laguerre polynomial expansion.[4,9] The Laguerre expansion was first proposed to solve the T. W. and some related equations by Ernst,[10] Barnsley and Cornille,[11] and Futcher *et al.*[2] A global existence theorem for solutions in L^1 of the T. W. equation was also shown to hold.[12,13] The convergence of the Laguerre expansion was proved for a family of initial conditions in the case of the T. W. and B. K. W. equations[11,14] and extended to a B. E. for Maxwell molecules with an angle dependent cross section.[15]

The aim of this paper is to carry out a systematic analysis of a class of models proposed by Ziff to which belong the T. W. and the B. K. W. models. In Sec. 1 we discuss some necessary conditions the kernels of the kinetic equations should satisfy in order to be actual B. E. Such conditions allow the *a priori* estimates related to particle number and energy conservation and asymptotic behavior (*H* theorem). In Sec. 2 we discuss the moment equations and the Laguerre polynomial expansion for the Ziff models. In Sec. 3 we first prove the existence and uniqueness of solutions in L^1. The equations for the Laguerre moments are examined and shown to have solutions in l^2 for initial conditions with not too large norm. As a consequence the corresponding Laguerre expansions do converge in L^2 due to an isometry with l^2. Finally using differential inequalities the approach to equilibrium is determined and the *H* theorem is justified.

1. KINETIC EQUATIONS

The Boltzmann equation for a homogeneous gas of identical particles in $d = 3$ space dimensions reads

$$\frac{\partial f}{\partial t}(v,t) = \frac{1}{4\pi}\int_{\mathbf{R}^3} d\mathbf{w}\int_0^{2\pi} d\epsilon\int_0^{\pi}\sin\chi d\chi \times B(g,\chi)[f(v',t)f(w',t) - f(v,t)f(w,t)], \tag{1.1}$$

where $\mathbf{v}$, $\mathbf{w}$; $\mathbf{v}'$, $\mathbf{w}'$ are the collision velocities, $g = |\mathbf{v}-\mathbf{w}| = |\mathbf{v}'-\mathbf{w}'|$ is the modulus of the relative velocity, χ and ϵ are the polar and azimuthal angle of the vector $\mathbf{v}'-\mathbf{w}'$, and $B(g,\chi)$ is the collision rate related to the center of mass scattering cross section σ by $B(g,\chi) = g\sigma(g,\chi)$.

Since Eq. (1.1) involves the kinematical difficulties of two particle collisions, equivalent equations depending, as the T. W. equation, only on the energy variables were considered. The general structure of such equations can be written according to Ziff[3]

$$\frac{\partial F}{\partial t}(x,t) = \int_0^\infty dy\int_0^\infty dz[P(y,z;x)F(y,t)F(z,t) - P(x,y;z)F(x,t)F(y,t)]. \tag{1.2}$$

The variables x,y,z are the kinetic energies of particles in the collision $y+z \rightarrow x+w$ where energy conservation requires $w = y+z-x$; $F(x,t)$ is the energy distribution function and the kernel $P(y,z;x)$ gives the probability for this collision to occur. Sufficient conditions on P for particle number and total energy conservation were analyzed by Ziff, who wrote the analytic expression of P corresponding to the original B. E. (1.1) for the B. K. W. model. For deterministic models P is linearly related to the cross section of the corresponding B. E. Ernst and Hendriks[4] exhibited an integral relation between P and the collision rate B in arbitrary space dimensions d for two classes of models specified by $B(g,\chi) = g^n\alpha(\chi)$ with $n = 0,2$ and $\alpha(\chi)$ arbitrary. The relation between P and B in space dimensions $d = 3$ and for arbitrary cross section was investigated by Barnsley and the author.[5] Choosing the relation between the distribution functions f and F according to

$$F(x,t) = 4\pi(2x)^{1/2}f((2x)^{1/2},t), \tag{1.3}$$

it was found that P can be written as

$$P(y,z;x) = \frac{\vartheta(x)\vartheta(y+z-x)\vartheta(y)\vartheta(z)}{(2y)^{1/2}(2z)^{1/2}} \times K(|y-z|,|y+z-2x|,y+z), \tag{1.4}$$

where K is linearly related to the collision rate B by a double integral and enjoys the symmetry property

$$K(a,b,c) = K(b,a,c). \tag{1.5}$$

As will be shown later Eq. (1.4) with the only constraint (1.5)

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on K guarantees particle number and energy conservation but does not guarantee momentum conservation. The latter is a hidden constraint and requires a particular functional structure of K. For isotropic cross sections namely $B = B(g)$ one has

$$K(a,b,c) = \frac{1}{2}\int_{\Lambda}^{\pi/2} d\tau\left[B\left(2\sqrt{c}\cos\frac{\tau}{2}\right) + B\left(2\sqrt{c}\sin\frac{\tau}{2}\right)\right], \tag{1.6}$$

where

$$\Lambda = \arcsin \max\left(\frac{a}{c}, \frac{b}{c}\right). \tag{1.7}$$

In order to include the models corresponding to the Boltzmann equation in dimensions $d \neq 3$ and eventually other stochastic kinetic models which do not correspond to momentum conserving B. E. in any dimension we replace (1.4) by

$$P(y,z;x) = \frac{\vartheta(x)\vartheta(y+z-x)\vartheta(y)\vartheta(z)}{p(y)p(z)} K(|y-z|,|y+z-2x|,y+z), \tag{1.8}$$

where K enjoys the symmetry (1.5). The only constraint on $p(.)$ is positivity. For B. E. in space dimensions d we have $p(y) = (2y)^{d/2-1}$. In order to exhibit the symmetry properties leading to the conservation laws and the H theorem we introduce a new distribution function

$$F(x,t) = \hat{F}(x,t)p(x), \tag{1.9}$$

a new kernel

$$\mathbb{P}(y,z|x,w) = K(|y-z|,|x-w|,y+z)\delta(y+z-x-w) \tag{1.10}$$

so that the kinetic equation (1.2) reads

$$p(x)\frac{\partial \hat{F}(x,t)}{\partial t} = \int_0^\infty dy\int_0^\infty dz\int_0^\infty dw\ \mathbb{P}(y,z|x,w) \times[\hat{F}(y,t)\hat{F}(z,t) - \hat{F}(x,t)\hat{F}(w,t)]. \tag{1.11}$$

On the kernel $\mathbb{P}$ one readily verifies the invariance under the exchange of the initial particles $y \leftrightarrow z$, of final particles $x \leftrightarrow w$,

$$\mathbb{P}(y,z|x,w) = \mathbb{P}(z,y|x,w) = \mathbb{P}(y,z|w,x) = \mathbb{P}(z,y|w,x) \tag{1.12}$$

and of initial and final particles among themselves, consequence of time reversal invariance

$$\mathbb{P}(y,z|x,w) = \mathbb{P}(x,w|y,z). \tag{1.13}$$

The last symmetry property was discussed in a less transparent form by Ziff[3] as "inverse collision symmetry" and by Futcher and Hoare[16] as "detailed balance condition."

Assuming that Eq. (1.11) has a solution and taking (1.12) and (1.13) into account we derive particle number and energy conservation and the asymptotic behavior in t as *a priori* estimates. Letting $\varphi(x)$ be a continuous function of x and assuming that $\hat{F}(x,t)p(x)\varphi(x)$ is integrable for $x\in[0,\infty[$ and that the integrand on the right hand side of (1.11) multiplied by $\varphi(x)$ is absolutely integrable with respect to all the energy variables and t, then using (1.12) and (1.13) we obtain

$$\begin{aligned}\frac{d}{dt}\int_0^\infty &\hat{F}(x,t)\varphi(x)p(x)dx \\ &= \frac{1}{4}\int_0^\infty dx\int_0^\infty dy\int_0^\infty dz\int_0^\infty dw\ \mathbb{P}(y,z|x,w) \\ &\quad\times[\hat{F}(y,t)\hat{F}(z,t) - \hat{F}(x,t)\hat{F}(w,t)] \\ &\quad\times[\varphi(x)+\varphi(w)-\varphi(y)-\varphi(z)].\end{aligned} \tag{1.14}$$

Among all continuous functions only the linear function satisfies the functional equation $\varphi(y) + \varphi(z) = \varphi(y+z-x) + \varphi(x)$ identically. As a consequence the only constants of motion of Eq. (1.11) are the first two moments $\mathscr{M}_0$, $\mathscr{M}_1$ of the solution

$$\mathscr{M}_n(t) = \int_0^\infty \hat{F}(x,t)x^n p(x)dx = \int_0^\infty F(x,t)x^n dx. \tag{1.15}$$

If we choose $\varphi(x) = \ln \hat{F}(x,t)$ then by the same procedure we show that

$$\frac{dH}{dt} \leqslant 0, \quad H = \int_0^\infty \hat{F}(x,t)\ln \hat{F}(x,t)p(x)dx. \tag{1.16}$$

If we assume that H is bounded below, then for $t\to\infty$ H must reach a constant value so that $dH/dt = 0$. As a consequence $\ln \hat{F}(x,t)$ has to be asymptotically a linear function of x,

$$\lim_{t\to\infty} \hat{F}(x,t) = \alpha e^{-\beta x}, \quad \lim_{t\to\infty} F(x,t) = \alpha p(x)e^{-\beta x}. \tag{1.17}$$

The normalization condition we choose to fix the positive constants α and β is

$$\alpha = \left(\int_0^\infty e^{-x}p(x)dx\right)^{-1}, \quad \beta = 1 \tag{1.18}$$

so that $\mathscr{M}_0 = 1$.

2. THE ZIFF MODELS AND THEIR PROPERTIES

The models proposed by Ziff are defined by Eq. (1.2) where the kernels depend on a continuous parameter and will be denoted by $P^{(m)}(y,z;x)$. The analytic structure of these kernels is specified by Eq. (1.8) with

$$p(x) = x^{m-1}, \quad K(a,b,c) = c^{2m-3}q^{(m)}[\tfrac{1}{2} - \tfrac{1}{2}\max(a/c,b/c)], \tag{2.1}$$

where $q^{(m)}$ is the incomplete beta function defined by

$$q^{(m)}(\lambda) = (m-1)\int_0^\lambda [u(1-u)]^{m-2}du. \tag{2.2}$$

The distribution function associated with $P^{(m)}$ will be denoted by $F^{(m)}$ and one can notice that $F^{(1)}$ and $F^{(3/2)}$ are the T. W. and B. K. W. distribution functions respectively, since $q^{(1)} = 1$ and $q^{(3/2)} = \arcsin\sqrt{\lambda}$, in agreement with (1.4) and (1.6) for $B = 1$. Cornille and Gervois[15,17] and Ernst and Hendriks[4] have shown that these models can be interpreted as momentum conserving B. E. in dimensions $d = 2m$.

A crucial property of the kernels $P^{(m)}(y,z;x)$ is that their integral on the variable x is independent of y and z. In fact as assumed by Ziff and proved in the Appendix one gets

$$\int_0^\infty P^{(m)}(y,z;x)dx = 1. \tag{2.3}$$

We assume $F^{(m)}(x,t)$ to satisfy the regularity condition of Sec. 1 so that according to (1.17), (1.18), and (2.1) its asymptotic limit is given by

$$\lim_{t\to\infty} F^{(m)}(x,t) = \frac{x^{m-1}}{\Gamma(m)} e^{-x} \tag{2.4}$$

and its zero order moment is equal to 1. Then Eq. (1.2) takes the form

$$\frac{\partial F^{(m)}}{\partial t}(x,t) + F^{(m)}(x,t) = \int_0^\infty dy \int_0^\infty dz\, P^{(m)}(y,z;x) F^{(m)}(y,t) F^{(m)}(z,t). \tag{2.5}$$

The moments of $P^{(m)}$ were assumed by Ziff after generalizing the results of the T. W. and B. K. W. models and allowed him to reconstruct the kernels themselves. In the Appendix, following the reverse procedure, given $P^{(m)}$ according to (1.8) and (2.1) we compute its moments and find in agreement with Ziff

$$\int_0^\infty P^{(m)}(y,z;x) x^n dx = \frac{(m)_n}{n+1} \sum_{j=0}^n \frac{y^j}{(m)_j} \frac{z^{n-j}}{(m)_{n-j}}, \tag{2.6}$$

where we used the notation $(m)_n = \Gamma(m+n)/\Gamma(m)$. The normalized moments $M_n^{(m)}(t)$ defined by

$$M_n^{(m)}(t) = \frac{\mathscr{M}_n^{(m)}(t)}{\mathscr{M}_n^{(m)}(\infty)} = \frac{1}{(m)_n} \int_0^\infty F^{(m)}(x,t) x^n dx \tag{2.7}$$

satisfy the following equations of motion:

$$\frac{dM_n^{(m)}}{dt} + M_n^{(m)} = \frac{1}{n+1} \sum_{j=0}^n M_j^{(m)} M_{n-j}^{(m)}, \tag{2.8}$$

as can be easily verified after multiplying (2.5) by x^n, integrating on x, and using (2.6) and (2.7).

A procedure to solve (2.8) with initial values $M_n^{(m)}(0)$ determined by the initial distribution has been derived in Ref. (11). However, in order to reconstruct the energy distribution at time t it is necessary to use a basis of orthogonal polynomials in $[0,\infty[$ with respect to a measure whose natural choice is $F^{(m)}(x,\infty)$. Such a basis is provided by the Laguerre polynomials of order $m-1$ for which we choose the standard normalization

$$L_n^{(m-1)}(x) = \frac{(m)_n}{n!}\, {}_1F_1(-n,m;x) = \sum_{k=0}^n \frac{(-x)^k}{k!} \binom{n+m-1}{n-k}, \tag{2.9}$$

where ${}_1F_1$ is the Kummer hypergeometric function. The orthogonality relations explicitly read

$$\int_0^\infty F^{(m)}(x,\infty) L_n^{(m-1)}(x) L_j^{(m-1)}(x) dx = \frac{(m)_n}{n!} \delta_{jn}. \tag{2.10}$$

We expand the distribution function in a series, whose convergence properties will be investigated later,

$$F^{(m)}(x,t) = F^{(m)}(x,\infty) \sum_{n=0}^\infty \Theta_n^{(m)}(t) L_n^{(m-1)}(x), \tag{2.11}$$

where the coefficients $\Theta_n^{(m)}(t)$, hereafter called Laguerre moments, are given by

$$\Theta_n^{(m)}(t) = \frac{n!}{(m)_n} \int_0^\infty F^{(m)}(x,t) L_n^{(m-1)}(x) dx. \tag{2.12}$$

The connection between the $\Theta_n^{(m)}$ and the normalized moments is found using (2.12), (2.9), and (2.7) and reads

$$\Theta_n^{(m)}(t) = \sum_{k=0}^n (-1)^k \binom{n}{k} M_k^{(m)}(t). \tag{2.13}$$

As a consequence (2.13) and (2.11) solve the initial value problem for $F^{(m)}(x,t)$. Nevertheless following Ernst and Hendriks[4] we notice the remarkable property of $\Theta_n^{(m)}(t)$ which satisfy the same differential equations as $M_n^{(m)}(t)$. In fact, as we prove in the Appendix, the Laguerre moments of $P^{(m)}(y,z;x)$ are given by

$$\int_0^\infty P^{(m)}(y,z;x) L_n^{(m-1)}(x) dx = \frac{(m)_n}{(n+1)!} \sum_{j=0}^n L_j^{(m-1)}(y) L_{n-j}^{(m-1)}(z) \frac{j!(n-j)!}{(m)_j (m)_{n-j}} \tag{2.14}$$

and consequently from (2.5) and (2.14) we obtain

$$\frac{d\Theta_n^{(m)}}{dt} + \Theta_n^{(m)} = \frac{1}{n+1} \sum_{j=0}^n \Theta_j^{(m)} \Theta_{n-j}^{(m)}. \tag{2.15}$$

3. EXISTENCE AND UNIQUENESS

Even though existence and uniqueness theorems are known for solutions in L^1 of the original B. E. for cutoff potentials[18] no such results are in general available for the recently proposed kinetic equations (1.2), be their origin deterministic or not. Moreover the solutions obtained via the Laguerre polynomial expansions for some of these models require existential theorems in L^2 spaces in order to be rigorously justified.

The T. W. model was quite intensively investigated. An existence and uniqueness theorem for continuous positive initial data in L^1 was first given using the method of monotone iterates.[19] The classical theorem on differential equations in Banach spaces, based on contraction mapping in its weak form, was used to prove the existence of a local weak solution in L^1 and the extension to any time was achieved by an iterative process based on estimates of the L^1 norm.[12] Finally existence and uniqueness of solutions in L^1 of the Tjon–Wu equation were shown to follow in the neatest way from a theorem of Brezis.[13] The same theorem allows one to select a class of initial data for which solutions in L^2 do exist.

In this section the above mentioned results are extended to the Ziff models. Dropping from now on the index m we write Eq. (2.5)

$$\frac{dF(t)}{dt} + F(t) = (SF)(t), \tag{3.1}$$

where S is the mapping defined by the right hand side of (2.5). Equation (3.1) is to be interpreted as a differential equation in a Banach space $L^1(0,\infty)$ whose norm we denote by

$$\|F(t)\|_1 = \int_0^\infty |F(x,t)| dx. \tag{3.2}$$

Lemma 1: S maps the unit ball of $L^1(0,\infty)$ into itself and is there uniformly Lipschitz.

In fact if $F \epsilon L^1(0,\infty)$ from (2.3) follows that

$$\|SF\|_1 \leqslant \|F\|_1^2. \tag{3.3}$$

Moreover if F and G belong to the unit ball of $L_1(0,\infty)$ then we have

$$\|SF-SG\|_1=\int_0^\infty dx\left|\int_0^\infty dy\int_0^\infty dz\,P(y,z;x)\times[F(y)F(z)-G(y)G(z)]\right|$$
$$=\int_0^\infty dx\left|\int_0^\infty dy\int_0^\infty dz\,P(y,z;x)\times[F(y)-G(y)][F(z)+G(z)]\right|$$
$$\leqslant\|F+G\|_1\|F-G\|_1\leqslant 2\|F-G\|_1. \quad (3.4)$$

To obtain this result the symmetry $P(y,z;x)=P(z,y;x)$ has been used.

The Brezis[20] theorem on differential equations in Banach spaces we need is the following.

Theorem 1: Let $\mathscr{C}$ be a closed convex of a Banach space and let S be a mapping of $\mathscr{C}$ into $\mathscr{C}$ such that

$$\|SF-SG\|\leqslant c\|F-G\|$$

for a constant c, then for $\forall F_0\in\mathscr{C}$ there exists a unique function $F(t)\in\mathscr{C}$ such that $F(t)$ is absolutely continuous in $[0,T]$ for any T, differentiable on $]0,T[$, and satisfies Eq. (3.1) with $F(0)=F_0$.

As a consequence the following result holds.

Theorem 2: Given any $F_0\epsilon\mathscr{C}$, where $\mathscr{C}$ is the unit ball of $L^1(0,\infty)$, then there is a unique solution $F(t)\epsilon\mathscr{C}$ of Eq. (3.1) with initial condition $F(0)=F_0$. Moreover if $F_0\epsilon\mathscr{C}_+$, where $\mathscr{C}_+$ is the intersection of $\mathscr{C}$ with the positive cone, then $F(t)\epsilon\mathscr{C}_+$.

It is important to notice that the physical solution belongs to the border of $\mathscr{C}_+$ defined by $\|F\|_1=1$. In fact if $F\epsilon\mathscr{C}_+$ then $\|SF\|_1=\|F\|_1^2$. Moreover we can write

$$F(t)=e^{-t}F(0)+\int_0^t e^{(\tau-t)}(SF)(\tau)d\tau \quad (3.5)$$

and due to the positivity condition for $F(t)$ we obtain

$$\|F(t)\|_1=e^{-t}\|F(0)\|_1+\int_0^t e^{(\tau-t)}\|F(\tau)\|_1^2d\tau. \quad (3.6)$$

The solution of (3.6) for $\|F(0)\|_1=1$ is $\|F(t)\|_1=1$. As a consequence $F(t)$ will satisfy the original equation (1.2).

Another relevant question concerns the convergence of the Laguerre polynomial expansion introduced in the previous section. For this purpose we consider the Hilbert space $L^2(0,\infty)$ with respect to the measure $\Gamma^{-1}(m)x^{m-1}e^{-x}$. Letting $\Phi(x,t)$ be the normalized energy distribution we write its Laguerre expansion as

$$\Phi(x,t)=\frac{F(x,t)}{F(x,\infty)}=\sum_{n=0}^\infty\left[\frac{n!}{(m)_n}\right]^{1/2}\hat{\Theta}_n(t)L_n^{(m-1)}(x), \quad (3.7)$$

where, in agreement with (2.11), the new Laguerre moments $\hat{\Theta}_n$ are related to the previous ones by

$$\hat{\Theta}_n=\left[\frac{(m)_n}{n!}\right]^{1/2}\Theta_n \quad (3.8)$$

and satisfy the differential equations

$$\frac{d\hat{\Theta}_n}{dt}+\hat{\Theta}_n=\frac{1}{n+1}\left[\frac{(m)_n}{n!}\right]^{1/2}\times\sum_{k=0}^n\left[\frac{k!(n-k)!}{(m)_k(m)_{n-k}}\right]^{1/2}\hat{\Theta}_k\hat{\Theta}_{n-k}. \quad (3.9)$$

Let us denote by $\|\cdot\|_2$ the norm in $L^2(0,\infty)$ with respect to the measure $\Gamma^{-1}(m)x^{m-1}e^{-x}$, namely,

$$\|\Phi(t)\|_2^2=\Gamma^{-1}(m)\int_0^\infty e^{-x}x^{m-1}\Phi^2(x,t)dx. \quad (3.10)$$

Let us also denote by $\hat{\Theta}(t)=(\hat{\Theta}_2(t),\hat{\Theta}_3(t),\ldots,\hat{\Theta}_n(t),\ldots)$ a vector of the Hilbert space l^2 with norm $\|\cdot\|$ given by

$$\|\hat{\Theta}(t)\|^2=\sum_{n=2}^\infty\hat{\Theta}_n^2(t). \quad (3.11)$$

We remark that the first two equations (3.9) for $n=0,1$ read

$$\frac{d\hat{\Theta}_0}{dt}+\hat{\Theta}_0=\hat{\Theta}_0^2,\quad \frac{d\hat{\Theta}_1}{dt}+\hat{\Theta}_1=\hat{\Theta}_0\hat{\Theta}_1. \quad (3.12)$$

If $F(x,t)$ is a solution of (2.5) corresponding to a positive initial condition with unit $L^1(0,\infty)$ norm, then we know that $\hat{\Theta}_0(t)=\Theta_0(t)=\|F(t)\|_1=1$. Moreover if $xF_1(x,t)$ also belongs to $L^1(0,\infty)$ then $\hat{\Theta}_1(t)$ also exists and has a constant value. Consistently with the asymptotic behavior that will be later rigorously justified we choose $\hat{\Theta}_1(t)$ to be zero.

Lemma 2: The series (3.7) establishes an isomorphism and an isometry between $L^2(0,\infty)$ and l^2.

In fact accounting for $\hat{\Theta}_0=1$, $\hat{\Theta}_1=0$ we have

$$\|\Phi(t)\|_2^2=1+\|\hat{\Theta}(t)\|^2. \quad (3.13)$$

As a consequence rather than investigating the L^2 containment of $\Phi(t)$, we investigate the l^2 containment of $\hat{\Theta}(t)$. The equation $\hat{\Theta}(t)$ satisfies can be written

$$\frac{d}{dt}\hat{\Theta}(t)+\hat{\Theta}(t)=(T\hat{\Theta})(t). \quad (3.14)$$

T is a mapping in l^2 defined by

$$T\hat{\Theta}=T_1\hat{\Theta}+T_2\hat{\Theta}, \quad (3.15)$$

where T_1 is the linear mapping

$$(T_1\hat{\Theta})_n=\frac{2}{n+1}\hat{\Theta}_n,\quad n\geqslant 2 \quad (3.16)$$

and T_2 is given by

$$(T_2\hat{\Theta})_n=\begin{cases}0, & 2\leqslant n<4\\ \dfrac{1}{n+1}\left[\dfrac{(m)_n}{n!}\right]^{1/2}\displaystyle\sum_{k=2}^{n-2}\left[\frac{k!(n-k)!}{(m)_k(m)_{n-k}}\right]^{1/2}\hat{\Theta}_k\hat{\Theta}_{n-k}, & n\geqslant 4.\end{cases} \quad (3.17)$$

In order to apply the Brezis theorem to Eq. (3.14) we need to estimate the l^2 norm of $T\hat{\Theta}$. Letting m_0 be the integer part of m and noticing that $(m)_k\geqslant(m_0)_k$ we have

$$\max_{2\leqslant k\leqslant n-2}\left[\frac{k!(n-k)!}{(m)_k(m)_{n-k}}\right]^{1/2}\leqslant\max_{2\leqslant k\leqslant n-2}\left[\frac{k!(n-k)!}{(m_0)_k(m_0)_{n-k}}\right]^{1/2}$$
$$=(m_0-1)!\max_{2\leqslant k\leqslant n-2}\left[\prod_{j=1}^{m_0-1}\frac{1}{(k+j)(n-k+j)}\right]^{1/2}$$
$$=\left[\frac{2!(n-2)!}{(m_0)_2(m_0)_{n-2}}\right]^{1/2}. \quad (3.18)$$

Indeed for any fixed j the minimum of $(k+j)(n-k+j)$ for $k\epsilon[2,n-2]$ is reached at any of the ends. As a consequence using the Schwarz inequality we have

$$\left|\sum_{k=2}^{n-2}\left[\frac{k!(n-k)!}{(m)_k(m)_{n-k}}\right]^{1/2}\hat{\Theta}_k\hat{\Theta}_{n-k}\right|$$
$$\leqslant\left[\frac{2!(n-2)!}{(m_0)_2(m_0)_{n-2}}\right]^{1/2}\sum_{k=2}^{n-2}|\hat{\Theta}_k||\hat{\Theta}_{n-k}|$$
$$\leqslant\left[\frac{2!(n-2)!}{(m_0)_2(m_0)_{n-2}}\right]^{1/2}\sum_{k=2}^{n-2}|\hat{\Theta}_k|^2$$
$$\leqslant\left[\frac{2!(n-2)!}{(m_0)_2(m_0)_{n-2}}\right]^{1/2}\|\hat{\Theta}\|^2. \tag{3.19}$$

The estimate of the norm of $T_2\hat{\Theta}$ follows from (3.17) and (3.19) and reads

$$\|T_2\hat{\Theta}\|^2=\sum_{n=4}^{\infty}(T_2\hat{\Theta})_n^2\leqslant c^2\|\hat{\Theta}\|^4, \tag{3.20}$$

where c is a constant given by

$$c^2=\sum_{n=4}^{\infty}\frac{1}{(n+1)^2}\frac{(m)_n}{n!}\frac{2!(n-2)!}{(m_0)_2(m_0)_{n-2}}. \tag{3.21}$$

When m is an integer then $m=m_0$ and the series can be explicitly summed according to

$$c^2=\frac{2}{m(m+1)}\sum_{n=4}^{\infty}\frac{1}{(n+1)^2}\times\left[1+\frac{2(m-1)}{n}+\frac{m(m-1)}{n(n-1)}\right]$$
$$=\frac{2}{m(m+1)}\left[\frac{(m-2)(m-3)}{2}\left(\frac{\pi^2}{6}-\frac{205}{144}\right)-\frac{(m-1)(5m-24)}{48}\right]. \tag{3.22}$$

The containment properties of T in l^2 are summarized by the following lemma.

Lemma 3: T maps the ball of l^2 of radius $R=1/3c$ into itself and is there uniformly Lipschitz. In fact if $\|\hat{\Theta}\|\leqslant R$ then from (3.15), (3.16), and (3.20) we obtain

$$\|T\hat{\Theta}\|\leqslant\|T_1\hat{\Theta}\|+\|T_2\hat{\Theta}\|\leqslant\tfrac{2}{3}\|\hat{\Theta}\|+c\|\hat{\Theta}\|^2\leqslant\tfrac{2}{3}R+cR^2=R. \tag{3.23}$$

Furthermore if $\hat{\Theta}$ and $\hat{\Psi}$ are in the ball of radius R, then

$$\|T\hat{\Theta}-T\hat{\Psi}\|\leqslant\tfrac{2}{3}\|\hat{\Theta}-\hat{\Psi}\|+c\|\hat{\Theta}+\hat{\Psi}\|\,\|\hat{\Theta}-\hat{\Psi}\|$$
$$\leqslant(\tfrac{2}{3}+2cR)\|\hat{\Theta}-\hat{\Psi}\|=\tfrac{4}{3}\|\hat{\Theta}-\hat{\Psi}\|. \tag{3.24}$$

In order to evaluate $T_2(\hat{\Theta}-\hat{\Psi})$ we have used the symmetry of the coefficients in (3.17) for $k\leftrightarrow n-k$ so that $\hat{\Theta}_k\hat{\Theta}_{n-k}-\hat{\Psi}_k\hat{\Psi}_{n-k}$ can be replaced by $(\hat{\Theta}_k-\hat{\Psi}_k)(\hat{\Theta}_{n-k}+\hat{\Psi}_{n-k})$.

Theorem 3: Given an initial condition $\hat{\Theta}(0)\epsilon l^2$ such that $\|\hat{\Theta}(0)\|\leqslant 1/(3c)$ there is a unique solution $\hat{\Theta}(t)\epsilon l^2$ of Eq. (3.14) for any $t>0$ such that $\|\hat{\Theta}(t)\|\leqslant 1/(3c)$.

The proof trivially follows from Theorem 1 and Lemma 3. From Lemma 2 follows that if $\Phi(0)$ belongs to the ball of $L^2(0,\infty)$ of radius $R=[1+1/9c^2]^{1/2}$ then the normalized solution at time $t,\Phi(t)$ defined by (3.7), also belongs to the same ball. As a consequence for this class of initial conditions the Laguerre expansion is convergent.

To conclude this section we show that $\|\hat{\Theta}(t)\|$ converges exponentially fast to 0 implying that the normalized solution converges exponentially fast to 1.

Theorem 4. Given an initial condition $\hat{\Theta}(0)\epsilon l^2$ such that $\|\hat{\Theta}(0)\|<1/(3c)$ then the following inequalities hold for the norm of the solution $\hat{\Theta}(t)$ of Eq. (3.14).

$$\frac{\|\hat{\Theta}(0)\|e^{-5t/3}}{1+\frac{3}{5}c\|\hat{\Theta}(0)\|(1-e^{-5t/3})}\leqslant\|\hat{\Theta}(t)\|\leqslant\frac{\|\hat{\Theta}(0)\|e^{-t/3}}{1-3c\|\hat{\Theta}(0)\|(1-e^{-t/3})}. \tag{3.25}$$

In fact scalar multiplying Eq. (3.14) by $\hat{\Theta}(t)$ and taking (3.16) and (3.20) into account we have

$$\left|\frac{1}{2}\frac{d}{dt}\|\hat{\Theta}(t)\|^2+\|\hat{\Theta}(t)\|^2\right|\leqslant\tfrac{2}{3}\|\hat{\Theta}(t)\|^2+c\|\hat{\Theta}(t)\|^3. \tag{3.26}$$

The following two differential inequalities obtained from (3.26),

$$\frac{1}{2}\frac{d}{dt}[e^{2t/3}\|\hat{\Theta}(t)\|^2]\leqslant ce^{-t/3}[e^{2t/3}\|\hat{\Theta}(t)\|^2]^{3/2} \tag{3.27}$$

and

$$\frac{1}{2}\frac{d}{dt}[e^{10t/3}\|\hat{\Theta}(t)\|^2]\geqslant-ce^{-5t/3}[e^{10t/3}\|\hat{\Theta}(t)\|^2]^{3/2}, \tag{3.28}$$

are readily solved to yield (3.25). As a consequence the asymptotic behavior of Φ is given by $\|\Phi(t)\|_2=1+O(e^{-2t/3})$.

APPENDIX

Ordinary moments

In order to prove (2.3) and (2.6) we first write the kernels $P^{(m)}(y,z;x)$ of the Ziff class, defined by (1.8), (2.1), and (2.2) in a more explicit way,

$$P^{(m)}(y,z;x)=\vartheta(y+z-x)\vartheta(x)\frac{(y+z)^{2m-3}}{(yz)^{m-1}}q^{(m)}(\lambda), \tag{A1}$$

where λ is a function of y,z,x such that for $z>y$

$$\lambda=\tfrac{1}{2}-\tfrac{1}{2}\max\left(\frac{|y-z|}{y+z},\frac{|y+z-2x|}{y+z}\right)=\begin{cases}\dfrac{x}{z+y}, & z>y>x\\[2mm] \dfrac{y}{z+y}, & z>x>y\\[2mm] 1-\dfrac{x}{z+y}, & x>z>y.\end{cases} \tag{A2}$$

Due to the summetry of $P^{(m)}(y,z;x)$ for $y\leftrightarrow z$ the kernel is then completely defined. The moments $\mathscr{P}_n^{(m)}(y,z)$ of $P^{(m)}(y,z;x)$ are given by

$$\mathscr{P}_n^{(m)}=\int_0^\infty x^nP^{(m)}(y,z;x)dx$$
$$=\frac{(y+z)^{2m-3}}{(yz)^{m-1}}\left\{\int_0^y x^nq^{(m)}\left(\frac{x}{z+y}\right)dx+q^{(m)}\left(\frac{y}{z+y}\right)\int_y^z x^ndx+\int_z^{z+y}x^nq^{(m)}\left(1-\frac{x}{z+y}\right)dx\right\}; \tag{A3}$$

changing integration variables we have

$$\mathscr{P}_n^{(m)} = \frac{(z+y)^{2m+n-2}}{(yz)^{m-1}}\left\{\int_0^{y/(z+y)}[\lambda^n+(1-\lambda)^n]q^{(m)}(\lambda)d\lambda + \frac{1}{n+1}\frac{z^{n+1}-y^{n+1}}{(z+y)^{n+1}}q^{(m)}\left(\frac{y}{z+y}\right)\right\}. \quad \text{(A4)}$$

Integrating by parts and accounting for $q^{(m)}(0)=0$ we find

$$\mathscr{P}_n^{(m)} = \frac{m-1}{n+1}\frac{(z+y)^{2m+n-2}}{(zy)^{m-1}} \times\int_0^{y/(z+y)}[(1-\lambda)^{n+1}-\lambda^{n+1}] \times\lambda^{m-2}(1-\lambda)^{m-2}d\lambda \quad \text{(A5)}$$

and the last integral is the difference of two incomplete beta functions. For $n=0$ we immediately verify that

$$\mathscr{P}_0^{(m)} = \int_0^\infty P^{(m)}(y,z;x)dx = (m-1)\frac{(z+y)^{2m-2}}{(zy)^{m-1}} \times\int_0^{y/(z+y)}[\lambda(1-\lambda)]^{m-2}d[\lambda(1-\lambda)] = 1. \quad \text{(A6)}$$

For arbitrary n and $m\geqslant 2$ integer we can write (A5) using the binomial expansion for $\lambda^{m-2}=[1-(1-\lambda)]^{m-2}$ and $(1-\lambda)^{m-2}$, respectively,

$$\begin{aligned}\mathscr{P}_n^{(m)} &= \frac{m-1}{n+1}\frac{(z+y)^{2m+n-2}}{(zy)^{m-1}}\sum_{k=0}^{m-2}(-1)^k\binom{m-2}{k}\int_0^{y/(z+y)}[(1-\lambda)^{m+n+k-1}-\lambda^{m+n+k-1}]d\lambda \\ &= \frac{m-1}{n+1}\frac{(z+y)^{2m+n-2}}{(zy)^{m-1}}\sum_{k=0}^{m-2}(-1)^k\binom{m-2}{k}\frac{1}{m+n+k}\left[1-\frac{z^{n+m+k}+y^{n+m+k}}{(z+y)^{n+m+k}}\right] \\ &= \frac{m-1}{n+1}\frac{1}{(zy)^{m-1}}\Big\{B(m-1,m+n)(z+y)^{2m+n-2}-\sum_{k=0}^{m-2}(-1)^k\binom{m-2}{k}\frac{1}{m+n+k} \\ &\quad\cdot(z^{m+n+k}+y^{m+n+k})(z+y)^{m-2-k}\Big\},\end{aligned} \quad \text{(A7)}$$

where $B(.,.)$ denotes the beta function. We can then write

$$\begin{aligned}\mathscr{P}_n^{(m)} &= \frac{m-1}{n+1}\frac{1}{(zy)^{m-1}}\left\{B(m-1,m+n)\sum_{j=m-1}^{n+m-1}\binom{2m+n-2}{j}y^{2m+n-2-j}z^j+R\right\} \\ &= \frac{(m-1)!}{n+1}(m+n-1)!\sum_{j=m-1}^{n+m-1}\frac{y^{m-1+n-j}z^{j-m+1}}{j!(2m+n-2-j)!}+\frac{m-1}{n+1}\frac{R}{(zy)^{m-1}} \\ &= \frac{1}{n+1}\frac{(n+m-1)!}{(m-1)!}\sum_{j=0}^{n}\frac{(m-1)!}{(j+m-1)!}\frac{(m-1)!}{(n-j+m-1)!}y^{n-j}z^j.\end{aligned} \quad \text{(A8)}$$

In fact we can show that R, which is a polynomial in z, y defined by

$$\begin{aligned}R &= B(m-1,m+n)\sum_{j=0}^{m-2}\binom{2m+n-2}{j}[y^{2m+n-2-j}z^j+z^{2m+n-2-j}y^j] \\ &\quad-\sum_{k=0}^{m-2}(-1)^k\binom{m-2}{k}\frac{1}{m+n+k}(z^{m+n+k}+y^{m+n+k})(z+y)^{m-2-k},\end{aligned} \quad \text{(A9)}$$

vanishes identically. We have simply to expand $(z+y)^{m-2-k}$ and write

$$\begin{aligned}R &= B(m-1,n+m)\sum_{j=0}^{m-2}\binom{2m+n-2}{j}y^{2m+n-2-j}z^j \\ &\quad-\sum_{k=0}^{m-2}(-1)^k\binom{m-2}{k}\frac{1}{m+n+k}\sum_{j=0}^{m-2}\binom{m-2-k}{j}y^{n+2m-2-j}z^j+(z\leftrightarrow y) \\ &= \sum_{j=0}^{m-2}y^{2m+n-2-j}z^j\left[B(m-1,n+m)\binom{2m+n-2}{j}-\sum_{k=0}^{m-2-j}(-1)^k\binom{m-2}{k}\binom{m-2-k}{j}\frac{1}{m+n+k}\right]+(z\leftrightarrow y).\end{aligned} \quad \text{(A10)}$$

Each of the coefficients in the last sum vanishes identically as one can easily check, accounting for the identity

$$\sum_{k=0}^{l}(-1)^k\binom{l}{k}\frac{1}{n+m+k} = B(l+1,n+m). \quad \text{(A11)}$$

We finally remark that the result proved for any integer $m\geqslant 2$ and valid for $m=1$ (as a direct calculation shows) can be analytically continued to any value of $m>1$ since $\mathscr{P}_n^{(m)}$, see (A5), is analytic for fixed n, y, z in a region containing the positive m axis beyond $m=1$.

Laguerre moments

The Laguerre moments $\mathscr{L}_n^{(m)}(y,z)$ of the kernel $P^{(m)}(y,z;x)$ can be easily computed starting from the relation

$$\frac{n!}{(m)_n}L_n^{(m-1)}(x) = \sum_{k=0}^{n}\binom{n}{k}\frac{(-x)^k}{(m)_k} \quad \text{(A12)}$$

and (A8), which combine to yield

$$\mathscr{L}_n^{(m)} = \frac{n!}{(m)_n} \int_0^\infty L_n^{(m-1)}(x) P^{(m)}(y,z;x) dx$$
$$= \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{1}{k+1} \sum_{j=0}^{k} \frac{y^j}{(m)_j} \frac{z^{k-j}}{(m)_{k-j}}. \quad \text{(A13)}$$

We then make use of the following identity:

$$\sum_{k=0}^{n} \binom{n}{k} \frac{1}{k+1} \sum_{j=0}^{k} a_j b_{k-j}$$
$$= \frac{1}{n+1} \sum_{k=0}^{n} \sum_{j=0}^{k} \binom{k}{j} a_j \sum_{l=0}^{n-k} \binom{n-k}{l} b_l, \quad \text{(A14)}$$

valid for any two sequences a_j, b_j. The proof of (A14) is immediate if we assume that a_j, b_j are moments of two measures, namely

$$a_j = \int \alpha^j dA(\alpha), \quad b_j = \int \beta^j dB(\beta). \quad \text{(A15)}$$

In this case in fact (A14) is verified if

$$\sum_{k=0}^{n} \binom{n}{k} \frac{1}{k+1} \sum_{j=0}^{k} \alpha^j \beta^{k-j}$$
$$= \frac{1}{n+1} \sum_{k=0}^{n} (1+\alpha)^k (1+\beta)^{n-k} \quad \text{(A16)}$$

and to show that (A16) holds we simply notice that the left hand side can be written

$$\sum_{k=0}^{n} \binom{n}{k} \frac{1}{k+1} \frac{\beta^{k+1} - \alpha^{k+1}}{\beta - \alpha}$$
$$= \sum_{k=0}^{n} \binom{n}{k} \frac{1}{\beta - \alpha} \int_\alpha^\beta x^k dx$$
$$= \frac{1}{n+1} \frac{(1+\beta)^{n+1} - (1+\alpha)^{n+1}}{(1+\beta) - (1+\alpha)}, \quad \text{(A17)}$$

which is identical to the right-hand side of (A16).

Finally using (A13) and (A14) we have

$$\mathscr{L}_n^{(m)} = \frac{1}{n+1} \sum_{k=0}^{n} \sum_{j=0}^{k} \frac{(-y)^j}{(m)_j} \binom{k}{j} \sum_{l=0}^{n-k} \frac{(-z)^l}{(m)_l} \binom{n-k}{l}$$
$$= \frac{1}{n+1} \sum_{k=0}^{n} \frac{k!}{(m)_k} L_k^{(m-1)}(y) \frac{(n-k)!}{(m)_{n-k}} L_{n-k}^{(m-1)}(z). \quad \text{(A18)}$$

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Mathematical problems of irreversible statistical mechanics for quantum systems. I: Analytic continuation of the collision and destruction operators by spectral deformation method

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We study some mathematical problems posed in nonequilibrium statistical mechanics and subdynamics theory developed by Prigogine and coworkers. We study in the superspace of the Hilbert–Schmidt operators the solution of the Liouville–von Neumann equation. The application in this frame of the spectral deformation methods yields expression of analytic continuations of a class of matrix elements of the resolvent of the Liouville–von Neumann operator, and this allows the analytic continuation of the collision and destruction operators. However, it is impossible to obtain simultaneously analytic continuation of the creation operator in this frame. The above results will be used in the second part of the article in order to study the pseudo-Markovian equation.

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1. INTRODUCTION

The theory of subdynamics was introduced by Prigogine, George, and Henin[1,2] in order to describe the irreversible process of the approach to equilibrium linked to the microscopic reversible dynamics. Very briefly speaking, the main idea of this theory is to find a suitable subspace of operators in which the total evolution generated by the Liouville–von Neumann operator reduces to a semigroup of operators related to the contributions of some singularities of the anayltic continuation of $[\psi(z) - z]^{-1}$ [where $\psi(z)$ is the so-called collision operator[3]] to the total evolution of the density matrix. The subspace π corresponding to poles near the orgin describes the asymptotic approach to equilibrium.

The main object of this paper is to develop a method of analytic continuation of the operators involved in this theory by considering only those solutions of the Liouville–von Neumann equation which are of Hilbert–Schmidt type. The general mathematical structure in which such analytic continuations exist is not well defined. In this respect, we have undertaken a preliminary study in a rather simplified mathematical structure. Here, we should point out that the space of the Hilbert–Schmidt operators contains all density matrices but it does not contain observables with continuous spectra. However, this space owing to its Hilbertian structure, allows the adaptation of the methods of analytic continuation previously elaborated in Hilbert spaces. These are essentially methods of analytic continuation of some matrix elements of the resolvent of a self-adjoint operator by use of an unbounded similarity between this self-adjoint operator and non-self-adjoint operators having spectra in the lower half-plane.

It is important to point out here that these methods only permit analytic continuation of some matrix elements of the resolvent of the Liouville operator and this limitation is the main reason it is impossible to obtain a projection operator corresponding to the subdynamics π in the Hilbertian structure. Nevertheless, they allow the construction of analytic continuation of the collision and destruction operators.

In the first part of this article we formulate the problem of the analytic continuation of the Liouville–von Neumann operator as a spectral deformation problem, and we deduce the analytic continuation of the collision operator $\psi(z)$ and the destruction operator $\mathscr{D}(z)$. In the second part we study the contributions of the complex singularities of $(\psi(z) - z)^{-1}$ analytically continued to the solution of the von Neumann equation, and we apply the formalism to the Lee model with a suitable cutoff.

The systems which we study here are quantum systems and their states are density matrices. The dynamics of these systems are described by Hamiltonians H (i.e., which are self-adjoint operators) acting on the space of wavefunctions $\mathscr{H}$ and the evolution of any density matrix ρ is given by

$$\rho(t) = e^{-itH}\rho e^{itH} = U_t\rho, \tag{1}$$

that is the solution of the Liouville–von Neumann equation

$$i\frac{\partial}{\partial t}\rho(t) = L\rho(t). \tag{2}$$

Here L is the Liouville operator

$$L\rho = [H,\rho] = H\rho - \rho H. \tag{3}$$

We should mention that the Liouville operator may be defined as the generator of the group of operators U_t [Eq. (1)] defined on the space of operators of Hilbert–Schmidt type $\mathscr{L}$ i.e., $Tr_{\mathscr{H}}(\rho^*\rho) < +\infty$. This space has a Hilbertian structure with the scalar product

$$\langle\rho,\rho'\rangle = Tr_{\mathscr{H}}(\rho^*\rho'). \tag{4}$$

L is then an unbounded self-adjoint operator with a dense domain, $\mathscr{D}(L)$.[4] Many results concerning the definition of L are given in[4]; we add here (proof in Appendix A) a complete characterization of the domain of L:

ρ belongs to the domain of L, $\mathscr{D}(L)$, if and only if $\rho\mathscr{D}(H) \subset \mathscr{D}(H)$ and $H\rho - \rho H$ extends to a Hilbert–Schmidt operator, $[H\rho - \rho H]^{\sim}$. (In the following $(\tilde{A})$ denotes the bounded extention of an operator A.)

For $t > 0$, $\rho(t)$ can be expressed as an inverse Laplace

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transform when $\rho(0)$ belongs to $\mathscr{D}(L)$:

$$U_t\rho = e^{-itL}\rho = \frac{1}{2i\pi}\int_{\mathscr{E}} dz\, e^{-izt}\frac{1}{L-z}\rho(0), \tag{5}$$

where $\mathscr{E}$ is line going from $(+\infty, +ic)$ to $(-\infty, +ic), c>0$.

A method developed by the Brussels school consists in studying the solution of the von Neumann equation (5) by using a decomposition of the resolvent $1/(L-z)$ through two orthocomplementary Hermitian projectors P and Q:

$$P + Q = 1. \tag{6}$$

Generally P projects onto the subspace of density matrices which are diagonal in a given orthonormal basis of $\mathscr{H}$. This yields the following decomposition of $1/(L-z)$:

$$(L-z)^{-1} = [P + \mathscr{C}(z)]\ [\psi(z) - z]^{-1}[P + \mathscr{D}(z)] + (QLQ - z)^{-1}Q, \tag{7}$$

where $\psi(z)$, $\mathscr{D}(z)$, and $\mathscr{C}(z)$, respectively called the collision, the destruction of correlations, and the creation of correlations operators,[3] are given by

$$\psi(z) = -PLQ(QLQ-z)^{-1}QLP, \tag{8}$$

$$\mathscr{D}(z) = -PLQ(QLQ-z)^{-1}, \tag{9}$$

$$\mathscr{C}(z) = -(QLQ-z)^{-1}QLP, \tag{10}$$

and PLP is generally taken as vanishing. From the above formulas it follows that the part $P\rho(t)$, denoted also $\rho_0(t)$, is given by

$$\rho_0(t) = P\rho(t) = -\frac{1}{2i\pi}\int_{\mathscr{E}} e^{-izt}[\psi(z)-z]^{-1}P\rho\, dz - \frac{-1}{2i\pi}\int_{\mathscr{E}} e^{-izt}[\psi(z)-z]^{-1}\mathscr{D}(z)Q\rho\, dz. \tag{11}$$

Another formula can be similarly derived for the "correlation part" $Q\rho(t)$ denoted also $\rho_c(t)$.

Remark: In order to make QLQ a self-adjoint operator and to define $\psi(z)$ as a family of bounded operators it is necessary to specify the projection P. It is sufficient to choose P projecting onto a subspace included in the domain of L, i.e., $R(\mathrm{P})\subseteq\mathscr{D}(L)$ (see Ref. 4).

The method then consists in the study of the contributions of the singularities of $[\psi(z)-z]^{-1}$ to the contour integral (11) supposing that $[\psi(z)-z]^{-1}$, $\mathscr{D}(z)$, and $\mathscr{C}(z)$ admit analytic continuations from the upper half-plane to the lower one. In this part of the article we will extend $\psi(z)$ to analytic family of operators $\psi^+(z)$ in some region D_0 of the lower half-plane. We will also extend analytically $\mathscr{D}(z)\,Q\rho(0)$ to D_0 for a class of initial states $\rho(0)$. The solutions of the equation

$$[\psi^+(z) - z]P\rho = 0$$

in D_0 that are isolated poles of $[\psi(z)-z]^{-1}$ in D_0 near the origin give the asymptotic irreversible evolution of $P\rho(t)$. If $\mathscr{C}(z)$ admit, also analytic continuation in D_0, then the $\tilde{\pi}$ projection operator can be constructed.[5] This hypothesis cannot be verified here as we shall show at the end of this section [see also (Ref. 4)], and only some matrix elements of $\mathscr{C}(z)$ can be analytically continued to D_0.

In order to construct analytic continuations of these operators we study the analytic continuation of the resolvent $(QLQ-z)^{-1}$. To this end we use the work of J. M. Combes[6] generalizing several techniques of analytic continuation of resolvents of self-adjoint operators.[7] It consists of looking for a non-self-adjoint operator $(QLQ)_d$ related to QLQ via unbounded similarity operators $\overline{U}$ and U such that

$$\langle\rho', (QLQ-z)^{-1}\rho\rangle = \langle\overline{U}\rho', [(QLQ)_d - z]^{-1}U\rho\rangle$$

for suitable ρ and ρ', so that for these matrix elements the domain of analyticity of $(QLQ-z)^{-1}$ is extended up to the continuous spectrum of $(QLQ)_d$ which lies in the lower half-plane.

Here it is important to stress the fact that this method is possible only when the Hamiltonian has absolutely continuous spectrum and the interaction has some mathematical properties. It implies also a selection of the class of initial states [via $Q\rho(0)$] as advocated by Prigogine and co-workers.[8]

2. SPECTRAL DEFORMATION OF THE LIOUVILLE OPERATOR

In this paragraph we study the problem of the similarity between the Liouville operator L and a non-self-adjoint operator L_d. In the next paragraph we shall study the problem of the similarity between the projection $(1-P)$ and a non-self-adjoint projection operator $(1-P_d)$ and apply the result to QLQ.

Let us formulate generally the problem of the spectral deformation of an operator via unbounded similarity.

Definition 1: Let A_1 be a closed densely defined operator in some Hilbert space $\mathscr{H}$, which generates a strongly continuous semigroup e^{itA_1} of type α_1.[9]

The operator A_2 is a spectral deformation of A_1 if: (1) A_2 generates a strongly continuous group e^{-itA_2} on a Hilbert space $\mathscr{H}_2$ of type α_2.

(2) There exists a pair of closed invertible operators $(\overline{U}, U)$ from $\mathscr{H}$, to $\mathscr{H}_2$ with dense domains and ranges such that

$$\langle\overline{U}\rho', U\rho\rangle = \langle\rho', \rho\rangle \tag{12}$$

for all ρ' in $\mathscr{D}(\overline{U})$ and ρ in $\mathscr{D}(U)$.

(3) $(A-z)^{-1}\mathscr{D}(U)\subset\mathscr{D}(U)$ for all $z\in\mathbb{C}$ with Im(z-) > max (α, α_2)

and

$$U(A_1 - z)^{-1}\rho = (A_2 - z)^{-1}U\rho. \tag{13}$$

Let us recall that a complex number z belongs to the resolvent set of A_1, $\rho(A_1)$, that is the complement of the spectrum of A_1, if $\mathrm{Im}(z) > \alpha_1$. We denote by $\sigma(A)$ the spectrum of the operator A.

We have the following lemma:

Lemma 1 (with the notation of definition 1): If A_2 is a spectral deformation of A_1 then

(i) $\rho\in\mathscr{D}(U)\Rightarrow e^{-iA_1t}\rho\in\mathscr{D}(U),\ t\geqslant 0$

and

$$Ue^{-itA_1}\rho = e^{-itA_2}U\rho. \tag{14}$$

(ii) $\rho\in\mathscr{D}(U)\cap\mathscr{D}(A)$ and $U\rho\in\mathscr{D}(A_2)\Rightarrow A_1\rho\in\mathscr{D}(U)$ and

$$A_2U\rho = UA_1\rho. \tag{15}$$

Proof: Let us use a slight modification of (5) to express $e^{-iA_1t}\rho$ for arbitrary ρ, $t>0$ and $c>\alpha_1$:[10]

$$e^{-iA_1t}\rho = \lim_{\omega\to\infty}\frac{1}{\omega}\int_0^\omega d\omega'\int_{\omega'+ic}^{-\omega'+ic} dz\, e^{-izt}\frac{1}{A_1-z}\rho.$$

By the closedness of U and using (13), we have

$$\lim_{\omega\to+\infty} U\Big(\frac{1}{\omega}\int_0^\omega d\omega'\int_{\omega'+ic}^{-\omega'+ic} e^{-izt}\frac{1}{A_1-z}\rho\Big) = e^{itA_2}U\rho,$$

for $c > \max(\alpha_1,\alpha_2)$. Using again the closedness of U we conclude the first part of the Lemma. If, now $\rho\in\mathscr{D}(U)\cap\mathscr{D}(A_1)$ and $U\rho\in\mathscr{D}(A_2)$, then we can differentiate the two sides of Eq. (14). The closedness of U ensures that $A_1\rho\in\mathscr{D}(U)$ and (15) follows. Q.E.D.

From (13) it follows that

$$\langle U^*\rho',(A_1-z)^{-1}\rho\rangle = \langle\rho',(A_2-z)U\rho\rangle. \tag{16}$$

As the domain of $\overline{U}$ is included in the range of U^*, $R(U^*)$ [for $U^*\supseteq\overline{U}^{-1}$, see (12)] then (16) implies that we have

$$\langle\rho',(A_1-z)^{-1}\rho\rangle = \langle\overline{U}\rho',(A_2-z)^{-1}U\rho\rangle, \tag{17}$$

for all $(\rho,\rho')\in\mathscr{D}(U)\times\mathscr{D}(\overline{U})$ and all z such that $\mathrm{Im}(z) > \max(\alpha_1,\alpha_2)$, and therefore $\langle\rho',(A_1-z)^{-1}\rho\rangle$ can be analytically continued to the resolvent sets of A_1 and A_2.

Let us return to our dynamical system described by the Hamiltonian H. If H_1 and H_2 are two spectral deformations of H via $(\overline{V}_1, V_1)$ and $(\overline{V}_2, V_2)$, respectively, our problem here is to deduce a spectral deformation of L. Define the semigroup

$$U_d(t)\rho = e^{-iH_1t}\rho e^{itH_2^*}. \tag{18}$$

It is easy to see that $U_d(t)$ is generated by the operator $-iL_d$ defined on a dense domain by

$$L_d\rho = [H_1\rho-\rho H_2^*]^\sim. \tag{19}$$

Now L_d is a spectral deformation of L. Let us give the proof of this result. Define the operators U' and $\overline{U}'$ by

$$U'(|\varphi\rangle\langle\psi|) = |V_1\varphi\rangle\langle V_2\psi|,$$

$$\overline{U}'(|\varphi'\rangle\langle\psi'|) = |\overline{V}_1\varphi'\rangle\langle\overline{V}_2\psi'|.$$

These are two invertible closable densely-defined operators which extend to operators U and $\overline{U}$ respectively, and satisfy

$$U\rho = (V_1\rho V_2^*)^\sim, \tag{20}$$

$$\overline{U}\rho = (\overline{V}_1\rho\overline{V}_2^*)^\sim, \tag{21}$$

for ρ in suitable domains (see Appendix B). The relation (12) can be verified directly. It remains to prove the third point of Definition 1. Consider (φ,ψ) in $\mathscr{D}(V_1)\times\mathscr{D}(V_2)$. By using the following relation (Ref. 11, p. 484) for a generator T of a semigroup of type α,

$$\frac{1}{T-z} = i\int_0^\infty e^{izt}e^{-iTt}\,dt,\quad \mathrm{Im}(z)>\alpha, \tag{22}$$

we obtain for L,

$$\frac{1}{L-z}|\varphi\rangle\langle\psi| = i\int_0^\infty dt e^{izt}|e^{-iHt}\varphi\rangle\langle e^{-iHt}\psi|. \tag{23}$$

On the other hand, by the closedness of U and Lemma 1, we have

$$U\Big(i\int_0^\tau dt\, e^{izt}|e^{-iHt}\varphi\rangle\langle e^{iHt}\psi|\Big)$$

$$= i\int_0^\tau dt\,|V_1e^{iHt}\varphi\rangle\langle V_2e^{-iHt}\psi|e^{izt}$$

$$= i\int_0^\tau dte^{izt}|e^{-iH_1t}V_1\varphi\rangle\langle e^{-H_2t}V_2\psi|, \tag{24}$$

and the last integral converges for Im (z) sufficiently great as $\tau\to\infty$. This implies that $(L-z)^{-1}|\varphi\rangle\langle\psi|$ belongs to $\mathscr{D}(U)$, and

$$U(L-z)^{-1}|\varphi\rangle\langle\psi| = (L_d-z)^{-1}U|\varphi\rangle\langle\psi|. \tag{25}$$

The above argument extends, without difficulty to any ρ in the domain of U by using its closedness and we obtain the following theorem:

Theorem 1: If H_1 and H_2 are two spectral deformations of H via $(V_1, \overline{V}_1)$ and $(V_2,\overline{V}_2)$ respectively, then the operator L_d given by

$$L_d\rho = [H_1\rho-\rho H_2^*]^\sim$$

is a spectral deformation of L via $(U,\overline{U})$ given by

$$U\rho = V_1\rho V_2^*$$

and

$$\overline{U}\rho = \overline{V}_1\rho\overline{V}_2^*.$$

3. ANALYTIC CONTINUATION OF THE COLLISION AND DESTRUCTION OPERATORS

We will investigate in this section analytic continuations of the collision operator. This means the extension of the domain of analyticity of the matrix elements

$$\langle\rho',\psi(z)\rho\rangle = \langle QLP\rho',(QLQ-z)^{-1}QLP\rho\rangle,$$

for all ρ and ρ', from the upper half-plane to some region in the lower half-plane through the real axis. It follows from the method developed in the preceding section that this is possible if there exists a spectral deformation $(QLQ)_d$ of QLQ with a continuous spectrum in the lower half-plane, and if $QLP\rho$ belongs to the domains of the operators U and $\overline{U}$ for all ρ. This is possible if the projection operator P satisfies some conditions, namely if P is transformed through the similarity U into a projection operator P_d such that $Q_dL_dQ_d$ is a spectral deformation of QLQ via $(U,\overline{U})$, where $Q_d = 1-P_d$. These conditions on P can be stated as follows: If P projects on a subspace contained in the domain of the operators U and $\overline{U}$, then the operator

$$P_d = (UPU^{-1})^\sim \tag{26}$$

defines a non-Hermitian projection operator. If moreover $R(P_d)\subset\mathscr{D}(L_d)$, then $Q_dL_dQ_d$ is a spectral deformation of the operator QLQ.

The above result is rather expected. It means that the analytic continuation problem cannot be solved for any representation P. We give the verification of the above properties in Appendix C.

Let us now compute the expressions of the analytic continuation of $\psi(z)$.

First we verify under the above conditions these two relations:

$$PLQ = U^{-1}P_dL_dQ_dU, \tag{27}$$

$$QLP = U^{-1}Q_dL_dP_dU \tag{28}$$

(the domains problems are discussed in Appendix C). Now by using the fact that $Q_dL_dQ_d$ is a spectral deformation of QLQ, i.e.,

$$U^{-1}(Q_dL_dQ_d - z)^{-1}U\rho = (QLQ - z)^{-1}\rho$$

for Im $(z) > 0$ sufficiently great, we get

$$U^{-1}P_dL_dQ_d(Q_dL_dQ_d - z)^{-1}Q_dL_dP_dU = PLQ\,(QLQ - z)^{-1}\,QLP,$$

or using a compact notation

$$\psi(z) = U^{-1}\psi_d(z)U,$$

where

$$\psi_d(z) = -P_dL_dQ_d(Q_dL_dQ_d - z)^{-1}Q_dL_dP_d.$$

[We similarly define the operators $\mathscr{D}_d(z)$ and $\mathscr{C}_d(z)$.] Now $U^{-1}\psi_d(z)U$ is analytic in $\rho(Q_dL_dQ_d)$ and coincides with $\psi(z)$ for Im $(z) > 0$; this yields the analytic continuation of $\psi(z)$. A similar result can be computed for $\mathscr{D}(z)Q\rho$ if ρ belongs to the domain of the operator U. Then we summarize our result in the following theorem:

Theorem 2: The collision operator $\psi(z)$ defined by (8) for Im $(z) > 0$ extends to an analytic family of bounded operators $\psi^+(z)$ in the resolvent set of the spectral deformation $Q_dL_dQ_d$ of QLQ. $\psi^+(z)$ is given by

$$\psi^+(z) = \begin{cases} \psi(z), & \mathrm{Im}(z) > 0, \\ U^{-1}\psi_d(z)U, & \mathrm{Im}(z) \leqslant 0 z \in \rho(Q_dL_dQ_d). \end{cases}$$

Thus destruction operator $\mathscr{D}(z)Q\rho$ defined by (9) has an analytic continuation $\mathscr{D}\,(z)Q\rho$ for ρ in the domain of U from the upper half-plane to the lower one in $\rho\,(Q_dL_dQ_d)$, given by

$$\mathscr{D}^+(z)Q\rho = \begin{cases} \mathscr{D}(z)Q\rho, & \mathrm{Im}(z) > 0, \\ = U^{-1}\mathscr{D}_d(z)UQ\rho, & \mathrm{Im}\,(z) \leqslant 0, z \in (Q_dL_dQ_d). \end{cases}$$

Corollary: The family $[\psi(z) - z]^{-1}$ has an analytic continuation from the upper half-plane to $\rho\,(L_d)\cap\rho(Q_dL_dQ_d)$, given by

$$[\psi(z) - z]^{-1} = \begin{cases} [\psi(z) - z]^{-1}, & \mathrm{Im}(z) > 0, \\ PU^{-1}\dfrac{1}{\psi_d(z) - z}U^{-1}P, & \mathrm{Im}(z) \leqslant 0, \\ (\psi^+(z) - z)^{-1} & z \in \rho(Q_dL_dQ_d)\cap\rho(L_d). \end{cases} \tag{29}$$

Remarks: We have constructed the analytic continuation of $[\psi(z) - z]^{-1}$. It remains to study the complex isolated singularities of $[\psi^+(z) - z]^{-1}$. Now the poles of $(\psi^+(z) - z)^{-1}$ are all points z in $\rho(Q_dL_dQ_d)$, where the "dispersion equation"

$$[\psi^+(z) - z]P\rho = 0, \tag{30}$$

or equivalently,

$$[\psi_d(z) - z]P_d\rho = 0, \tag{30'}$$

has a nonvanishing solution $P_d\rho$; these $z \in \mathbb{C}$ which are solutions of the dispersion equation are exactly eigenvalues of L_d for the eigenvectors

$$\rho_z = P_d\rho_z + \mathscr{C}_d(z)P_d\rho_z \tag{31}$$

(see Appendix D).

It follows that the operator $\mathscr{C}(z)$ may not admit an analytic continuation similar to the collision and destruction operators. In fact, one can easily see that $U^{-1}\mathscr{C}_d(z)U$ coincide with $\mathscr{C}(z)$ for Im $(z) > 0$ and sufficiently great. However, this operator may not be defined in the lower half-plane, and surely not for the solution of the dispersion Eq. (30); for in this case we get from (31) and (15),

$$L\,U^{-1}\rho_z = U^{-1}L_d\rho_z = U^{-1}z\rho_z = zU^{-1}\rho_z,$$

that is, $U^{-1}\rho_z$ would be an eigenfunction of L with a nonreal eigenvalue z. This contradicts the self-adjointness of L and $\mathscr{C}_d(z)\rho \notin \mathscr{D}(U^{-1}) = R\,(U)$. Therefore we conclude that in the Hilbert-Schmidt space, it is impossible to obtain rigorously a $\tilde{\pi}$ projection operator with spectral deformation methods. All we can do is to continue analytically matrix elements of $\mathscr{C}(z)$ in the lower half-plane.

In the next paper we shall study the contribution to the diagonal part $P\rho(t)$ of the poles of $(\psi^+(z) - z)^{-1}$ in order to obtain the "pseudo-Markovian" kinetic equation

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APPENDIX A

The following conditions are equivalent:

(1) $\rho \in \mathscr{D}(L)$,

(2) $\rho\mathscr{D}(H) \subset \mathscr{D}(H)$ *and* $(H\rho - \rho H)$ *extends to a Hilbert–Schmidt operator. In this case* $L\rho = (H\rho - \rho H)^{\sim}$ for $\rho \in \mathscr{D}(L)$ where $\sim$ denotes the bounded extension.

Proof: It has been shown[12] that $\rho \in \mathscr{D}(L)$ if and only if there exists a constant C_ρ such that

$$\|[(U_t - 1)/t\,]\rho\|_2 \leqslant c_\rho$$

for all t. Let $\{\psi_i\}$ be an orthonormal base in $\mathscr{D}(H)$; then,

$$\left\|\left(\frac{U_t - 1}{t}\right)\rho\right\|_2^2 = \sum_i \|[(U_t - 1)/t\,]\rho\psi_i\|^2.$$

On the other hand, it is easy to see that

$$\frac{d}{dt}(U_t\rho)\psi = U_t\,[H,\rho]\psi$$

for all $\psi \in \mathscr{D}(H)$. Then,

$$\frac{U_t - 1}{t}\rho\psi_i = (1/t)\int_0^t ds\, e^{-isH}[H,\rho]e^{ish}\psi_i.$$

This implies the following inequaltity:

$$\left\|\left(\frac{U_t - 1}{t}\right)\rho\psi_i\right\|^2 \leqslant \frac{1}{t}\int_0^t ds\,\|[H,\rho]e^{isH}\psi_i\|^2,$$

as $\{e^{isH}\psi_i\}$ is an orthonormal basis for all s; then by the Lebesgue dominated convergence theorem we get

$$\left\|\left(\frac{U_t - 1}{t}\right)\rho\right\|_2^2 \leqslant \sum_i \frac{1}{t}\int_0^t ds\,\|[H,\rho]e^{isH}\psi_i\|^2 = \frac{1}{t}\int_0^t ds\|\,[H,\rho]\,\|_2^2 = \|[H,\rho]\|_2^2.$$

This proves that $2 \Rightarrow 1$. The converse was proved in Ref. 4.

APPENDIX B

If the domain of U^* is the set of ρ such that $R(\rho) \subset \mathscr{D}(V_1^*)$ and $V_1^* \rho V_2$ extends to a Hilbert–Schmidt operator, then

$$U^* \rho = [V_1^* \rho V_2]^{\sim}.$$

Similarly, we have for $\bar{U}^*$,

$$\bar{U}^* \rho = [\bar{V}_1^* \rho \bar{V}_2]^{\sim}.$$

Proof: $U^* = U'^*$ by a theorem of von Neumann.

Let $\rho \in \mathscr{D}(U^*)$, then for all $(\phi,\psi) \in \mathscr{D}(V_1) \times \mathscr{D}(V_2)$ we have

$$\begin{aligned}\langle (|V_1 \varphi\rangle\langle V_2\psi|), \rho\rangle &= \mathrm{Tr}(|V_2\psi\rangle\langle V_1\varphi|\rho)\\ &= \langle V_1\varphi, \rho V_2\psi\rangle\\ &= \mathrm{Tr}(|\psi\rangle\langle\varphi|U^*\rho)\\ &= \langle\varphi, U^*\rho\psi\rangle.\end{aligned}$$

Thus $\rho V_2 \psi \in \mathscr{D}(V^*)$ and $V_1^* \rho V_2 \psi = U^* \rho\psi$. Let us prove the converse. If ρ is such that $R(\rho V_2) \subseteq \mathscr{D}(V_1^*)$ and $V_1^* \rho V_2 \in \mathscr{L}$, then for all $\varphi \in \mathscr{D}(V_1)$ and $\psi \in \mathscr{D}(V_2)$ we have

$$\begin{aligned}\langle (|\varphi\rangle\langle\psi|), [V_1^*\rho V_2]^{\sim}\rangle &= \langle \varphi, V_1^* \rho V_2 \psi\rangle\\ &= \langle V_1\varphi, \rho V_2\psi\rangle\\ &= \langle (|V_1\varphi\rangle\langle V_2\psi|), \rho\rangle\\ &= \langle U'(|\varphi\rangle\langle\psi|), \rho\rangle.\end{aligned}$$

Thus $\rho \in \mathscr{D}(U^*)$ and $U^*\rho = [V_1^* \rho V_2]^{\sim}$. Let us finally remark that if $[V_1^*\rho V_2]^{\sim}$ is Hilbert–Schmidt then $\rho V_2 \psi \in \mathscr{D}(V_1^*), \psi \in \mathscr{D}(V_2)$. This implies by the density of $R(V_2)$ and the closedness of V_1^* that $\rho\psi \in \mathscr{D}(V_1^*)$ for all $\psi \in \mathscr{H}$.

Corollary: If $\rho \in \mathscr{D}(U)$ then $R(\rho) \subset \mathscr{D}(V_1)$ and $V_1 \rho V_1^*$ extends to a Hilbert–Schmidt operator. In this case U is given by

$$U\rho = [V_1 \rho V_1^*]^{\sim}.$$

Similarly, for U

$$\bar{U}\rho = [\bar{V}_1\rho\, \bar{V}_1^*]^{\sim}, \quad \rho \in \mathscr{D}(\bar{\mathrm{U}}).$$

Proof: Let $(\varphi,\psi) \in \mathscr{D}(V_1^*) \times \mathscr{D}(V_2^*$ and $\rho \in \mathscr{D}(U)$. Then,

$$\begin{aligned}\langle U^*(|\varphi\rangle\langle\psi|), \rho\rangle &= \langle (|V_1^*\varphi\rangle\langle V_2^*\psi|, \rho\rangle\\ &= \langle V_1^*\varphi, \rho V_2^*\psi\rangle\\ &= \langle (|\varphi\rangle\langle\psi|), \mathrm{U}\rho\rangle\\ &= \langle\varphi, (U\rho)\psi\rangle.\end{aligned}$$

Thus $\rho V_2^* \psi \in \mathscr{D}(V_1)$ and $V_1 \rho V_2^* \psi = (U\rho)\psi$.

APPENDIX C

(1) UPU^{-1} extends to a projection operator P_d: it is sufficient to see that UPU^{-1} is bounded. In fact PU^{-1} is bounded for $(PU^{-1})^* \supset U^{*-1}P = \bar{U}P$ and $\bar{U}P$ is bounded by the closed graph theorem. Therefore UPU^{-1} is bounded for $R(P) \subset \mathscr{D}(U)$.

(2) $Q_d L_d Q_d$ is the spectral deformation of QLQ. It can be easily seen that $Q_d L_d Q_d$ is densely defined and closed when $R(P_d) \subset \mathscr{D}(L_d)$ and $R(P_d^*) \subset \mathscr{D}(L_d^*)$. In this case $Q_d L_d Q_d$ generates a semigroup as a result of the stability of a generator through bounded perturbation (Ref. 11, p. 495). To prove Property 3 of the definition, let $\rho \in \mathscr{D}(U)$ and denotes

$$\rho' = (QLQ - z)^{-1}\rho.$$

We have

$$(L - z)\rho' = [QLQ - z]\rho' + PLP' - LP\rho'.$$

Now $(L - z)$ belongs to $\mathscr{D}(U)$. In fact $(QLQ - z)\rho' = \rho$ and $PL\rho'$ are in $\mathscr{D}(U)$. Moreover, $LP\rho'$ is also in $\mathscr{D}(U)$ as a result of the Lemma 1 $[UP\rho = P_d UP\rho \in \mathscr{D}(L_d)]$. Thus $\rho \in (L - z)^{-1}\mathscr{D}(U) \subset \mathscr{D}(U)$. Applying Lemma 1, we get

$$(Q_d L_d Q_d - z)U\rho' = U(QLQ - z)\rho'.$$

Thus

$$U(QLQ - z)^{-1}\rho = (Q_d L_d Q_d - z)^{-1}\, U\rho$$

$\mathrm{Im}(z) > 0$ sufficiently great and this completes the proof.

(3) It follows from above that $QLP\rho \in \mathscr{D}(U)$ and $UQLP\rho = Q_d L_d Q_d UP\rho$. This verifies (27). Equation (28) is verified similarly.

APPENDIX D

The poles of $[\psi^+(z) - z]^{-1}$ in the lower half-plane are poles of $[\psi_d(z) - z]^{-1}$, and these are poles of $(L_d - z)^{-1}$ necessarily, i.e., isolated eigenvalues of L_d.

We shall show that $z_0 \in \rho(Q_d L_d Q_d)$ is an eigenvalue of L_d if and only if the equation

$$[\psi_d(z_0) - z_0]P_d\rho = 0$$

has a nonvanishing solution.

Let $\rho \neq 0$ be an eigenfunction of L_d for the eigenvalue z_0:

$$L_d\rho = z_0\rho. \tag{D1}$$

This last equation is equivalent to the following two equations:

$$P_d L_d P_d \rho + P_d L_d Q_d \rho = z_0 P_d \rho, \tag{D2}$$

$$Q_d L_d \mathrm{P}_d \rho + Q_d L_d Q_d \rho = z_0 Q_d \rho. \tag{D3}$$

Let us multiply (D2) by $(Q_d L_d Q_d - z)^{-1}$ on the left, use the equation $(T - z)^{-1} T \subset 1 + z(T - z)^{-1}$ for the resolvent of an operator T, and pass to the limit $z \rightarrow z_0$. We get easily the following equations:

$$\psi_d(z_0) P_d \rho = z_0 P_d \rho, \tag{D4}$$

$$Q_d \rho = \mathscr{C}_d(z_0) P_d \rho. \tag{D5}$$

This implies that (D4) has a nonvanishing solution $P_d\rho$, otherwise, $Q_d\rho$ will be vanishing and this contradicts equation (D1).

Let now z_0 to be a point in $\rho(Q_d L_d Q_d)$ such that (D4) has a nonvanishing solution and let $\rho = P_d\rho + \mathscr{C}_d(z_0)P_d\rho$. Thus we have

$$P_d L_d \rho = P_d L_d P_d \rho + P_d L_d Q_d \rho. \tag{D6}$$

Substituting (D5) in (D6) we get

$$P_d L_d \rho = z_0 P_d \rho. \tag{D7}$$

On the other hand, we have

$$\begin{aligned}Q_d L_d \rho &= Q_d L_d P_d \rho + Q_d L_d Q_d \rho\\ &= Q_d L_d P_d \rho - Q_d L_d Q_d (Q_d L_d Q_d - z_0)^{-1} Q_d L_d P_d \rho\\ &= z_0 (Q_d L_d Q_d - z_0)^{-1} Q_d L_d P_d \rho\\ &= z_0 \mathscr{C}_d(z_0)\rho = z_0 Q_d \rho.\end{aligned} \tag{D8}$$

Thus, by adding (D7) and (D8) we get

$$L_d \rho = z_0 \rho,$$

and this prove that z_0 is an eigenvalue of L_d.

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Mathematical problems of irreversible statistical mechanics for quantum systems. II: On the singularities of $(\Psi(z) - z)^{-1}$ and the pseudo-Markovian equation. Application to Lee model

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We study in the frame of the superspace of the Hilbert–Schmidt operators the contributions of some complex singularities of the analytic continuation of $(\Psi(z) - z)^{-1}$ to the diagonal part of the solution of the Liouville–von Neumann equation. Under some conditions, the $\tilde{\theta}$ operator of the pseudo-Markovian master equation can be explicitly constructed. It is necessary to specify the diagonal representation and the class of initial conditions having regularity properties. This Hilbertian structure does not allow the construction of a closed subspace which reduces the Liouville–von Neumann operator L, giving an exact irreversible subdynamics; more elaborate mathematical structures are therefore necessary. The above methods are illustrated in the case of the Lee model.

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1. INTRODUCTION

In the first part of this article (referred to here as I)[1] we have given expressions of analytic continuations of the collision and destruction operators. These operators play an important role in the theory of the nonequilibrium statistical mechanics,[2] based on the study of the solution of the Liouville–von Neumann equation for $t > 0$:

$$U_t\rho = -\frac{1}{2i\pi}\int_{\bar{C}} e^{-izt}\frac{1}{L-z}\rho\, dz, \tag{1}$$

where L is the Liouville operator acting on a density matrix ρ as follows:

$$L\rho = H\rho - \rho H,$$

and H is the Hamiltonian of the system. For this purpose, one introduces the decomposition of the resolvent of L by two orthocomplementary projection operators P and $Q = 1 - P$:

$$(L - z)^{-1} = [P + \mathscr{C}(z)](\Psi(z) - z)^{-1}[P + \mathscr{D}(z)] + (QLQ - z)^{-1}Q, \tag{2}$$

where

$$\Psi(z) = -PLQ(QLQ - z)^{-1}QLP, \tag{3}$$

$$\mathscr{D}(z) = -PLQ(QLQ - z)^{-1}Q, \tag{4}$$

$$\mathscr{C}(z) = -Q(QLQ - z)^{-1}QLP, \tag{5}$$

which are called respectively collision, destruction of correlations, and creation of correlations operators.

In this theory, analytic continuations of $\Psi(z)$, $\mathscr{D}(z)$, and $\mathscr{C}(z)$, respectively $\Psi^\dagger(z)$, $\mathscr{D}^\dagger(z)$, and $\mathscr{C}^\dagger(z)$, in the lower half-plane together with the solutions of the equation

$$[\Psi^\dagger(z) - z]P\rho = 0 \tag{6}$$

yield complex poles and provide contributions to (1) which allows separation of the evolution into irreversible subdynamics.

We have tried to study the mathematical problems posed by this theory in the frame of the space of the Hilbert–Schmidt operators. The limitations of this structure have been pointed out in the first part of this article. There, we have used a method of spectral deformation which gives expressions of analytic continuation $\Psi^\dagger(z)$ and $\mathscr{D}^\dagger(z)$, and we have shown that the operators

$$\Psi^\dagger(z) = U^{-1}P_dL_dQ_d(Q_dL_dQ_d - z)^{-1}Q_dL_dP_dU, \tag{7}$$

$$\mathscr{D}^\dagger(z) = U^{-1}P_dL_dQ_d(Q_dL_dQ_d - z)^{-1}U, \tag{8}$$

define analytic continuations of $\Psi(z)$ and $\mathscr{D}(z)$ from the upper half-plane to the lower one. Here $Q_dL_dQ_d$ is a spectral deformation of QLQ. Let us recall briefly and heuristically the above notions.

A non-self-adjoint operator H_1, with a spectrum in the lower half-plane, is a spectral deformation of a self-adjoint operator H if there exist two (unbounded) operators $\bar{V}$ and V such that

$$\langle \bar{V}\Psi, V\varphi\rangle = \langle\Psi,\varphi\rangle, \tag{9}$$

$$V^{-1}(H_1 - z)^{-1}V\Psi = (H - z)^{-1}\Psi, \tag{10}$$

for $\mathrm{Im}(z) > 0$ and sufficiently great.

If now, H_1 and H_2 are two spectral deformations of H via $(\bar{V}_1V_1)$ and $(\bar{V}_2V_2)$, then we may construct a spectral deformation of L, namely,

$$L_d\rho = [H_1\rho - \rho H_2^*]^\sim, \tag{11}$$

via two unbounded operators $\bar{U}$ and U given in terms of $(\bar{V}_1, V_1)$ and $(\bar{V}_2, V_2)$. The operators L and L_d act on the space of the Hilbert–Schmidt operators, denoted $\mathscr{L}$. Then, introducing the projection $P_d = UPU^{-1}$, we have shown that $Q_dL_dQ_d$ is a spectral deformation of QLQ, where $Q = 1 - P$ and $Q_d = 1 - P_d$.

In the next paragraph, we study the contributions of the singularities which result from the solutions of the dispersion equation (6) to the diagonal part of the density matrix given by

$$P\rho(t) = -\frac{1}{2i\pi}\int_{\bar{C}} e^{-izt}\frac{1}{\Psi(z) - z}P\rho\, dz - \frac{1}{2i\pi}\int_{\bar{C}} e^{-izt}\frac{1}{\Psi(z) - z}\mathscr{D}(z)Q\rho\, dz. \tag{12}$$

2. CONTRIBUTIONS TO THE DIAGONAL PART OF THE DENSITY MATRIX

Let z_0 be an isolated singularity of $[\Psi^\dagger(z) - z]^{-1}$; then z_0 is an isolated singularity of $(\Psi_d - z)^{-1}$, and also an isolated singularity of $(L_d - z)^{-1}$. If π_{z_0} is the projection operator

$$\pi_{z_0} = -\frac{1}{2i\pi}\int_{\gamma_{z_0}} dz \frac{1}{L_d - z}, \tag{13}$$

then the residue of $(\Psi^\dagger(z) - z)^{-1}$ is $-\widetilde{A}_0$, with

$$\widetilde{A}_0 = PU^{-1}A_0UP, \tag{14}$$

where

$$A_0 = P_d\pi_{z_0}P_d \tag{14'}$$

if z_0 is a pole; then π_{z_0} is of finite rank and the same is true for A_0. We shall study here the contributions of N poles of order one $(z_1,z_2,...,z_N)$, to the diagonal part $P\rho(t)$. For general poles of order $\hbar$, analogous but more complicated conditions can be established similarly as in Ref. 3. We consider only poles such that the ranges of A_i, $R(A_i)$ are linearly independent. Let $\mathscr{F}$ be the direct sum of these subspaces:

$$\mathscr{F} = \bigoplus_{i=1}^{N} R(A_i). \tag{15}$$

Let $\{F_i\}_{i=1}^N$ be the complementary projectors on $R(A_i)$, not necessarily Hermitians, satisfying

$$\sum_i F_i = 1_{\mathscr{F}}, \tag{16}$$

$$F_iF_j = \delta_{i,j}F_i; \tag{17}$$

one can define the operator θ in $\mathscr{F}$ by

$$\theta = \sum_i z_iF_i. \tag{18}$$

It follows from (12) that the contributions of these singularities to $Pe^{-itL}P\rho$, which we denote by $\tilde{\rho}_{0,0}(t)$ give

$$\tilde{\rho}_{0,0}(t) = PU^{-1}e^{-i\theta t}AUP\rho, \tag{19}$$

where A is defined by

$$A = \sum_{i=1}^{N} A_i. \tag{20}$$

Using the relation $P_d = UPU^{-1}$, we can easily see that the family of operators $\widetilde{F}_1,...,\widetilde{F}_N$, defined by

$$\widetilde{F}_i = PU^{-1}F_iUP, \tag{21}$$

is a family of projection operators of $P\mathscr{L}$, and we have

$$\widetilde{F}_i\widetilde{F}_j = \delta_{i,j}\widetilde{F}_i. \tag{22}$$

Let $\widetilde{\mathscr{F}}$ be a direct sum of $R(\widetilde{F}_i)$:

$$\widetilde{\mathscr{F}} = \bigoplus_{i=1}^{N} R(\widetilde{F}_i), \tag{23}$$

and let $\tilde{\theta}$ be the bounded operator in $\widetilde{\mathscr{F}}$ defined by

$$\tilde{\theta} = \sum_i z_i\widetilde{F}_i. \tag{24}$$

Thus we have

$$\tilde{\rho}_{0,0}(t) = e^{-i\tilde{\theta}t}\widetilde{A}\rho, \tag{25}$$

where $\widetilde{A}$ is given by

$$\widetilde{A} = PU^{-1}AUP = \sum_i \widetilde{A}_i \tag{26}$$

with

$$R(\widetilde{A}_i) = R(\widetilde{F}_i). \tag{27}$$

$\rho'(t) = e^{-i\tilde{\theta}t}\rho'$ is the solution of the differential equation in $\widetilde{\mathscr{F}}$:

$$i\frac{\partial}{\partial t}\rho'(t) = \tilde{\theta}\rho'(t) \tag{28}$$

for all $\rho' \in \widetilde{\mathscr{F}}$.

Thus $\tilde{\rho}_{0,0}(t)$ is a solution of the Eq. (28). In a similar way, we can extract from (12) the contributons of the poles $\{z_1,...,z_N\}$ to $Pe^{-itL}Q\rho$ for all $Q\rho$ in $\mathscr{D}(U)$, which we denote by $\tilde{\rho}_{0,c}(t)$:

$$\begin{aligned}\tilde{\rho}_{0,c}(t) &= \sum_i e^{-iz_it}PU^{-1}A_i\mathscr{D}_d(z_i)UQ\rho \\ &= PU^{-1}e^{-i\theta t}BUQ\rho,\end{aligned} \tag{29}$$

where B is the operator given by

$$B = \sum_i A_i\mathscr{D}_d(z_i). \tag{30}$$

$\tilde{\rho}_{0,c}(t)$ can also be written as

$$\tilde{\rho}_{0,c}(t) = e^{-i\tilde{\theta}t}\widetilde{B}Q\rho, \tag{31}$$

where $\widetilde{B}$ is given by

$$\widetilde{B} = U^{-1}BU. \tag{32}$$

This gives the contributions of these poles to $Pe^{-itL}Q\rho$ for all $\rho \in \mathscr{D}(U)$:

$$\tilde{\rho}_0(t) = e^{-i\tilde{\theta}t}[\widetilde{A} + \widetilde{B}]\rho. \tag{33}$$

If now $R(B) \subseteq R(A)$—that is equivalent to the condition $N(A^*) \subseteq N(B^*)$—then by the Lagrange's multipliers theorem there exists an operator D^* such that $B^* = D^*A^*$, i.e., $B = AD$. Thus, we have

$$\tilde{\rho}_0(t) = e^{-i\tilde{\theta}t}\widetilde{A}[P + \widetilde{D}]\rho, \tag{34}$$

where $\widetilde{D} = U^{-1}DU$. That is true in particular if $\{R(A_i^*)\}$, $i = 1,...,N$, are linearly independent [When $R(A_i)$ and $R(A_i^*)$ are two set of linearly independent subspaces we shall say that the $\{z_i\}$ verify the direct sum property.], and G_i^* is the projection operator on $R(A_i^*)$ along $\oplus_{j\neq i} R(A_j^*)$, then D is given by

$$D = \sum_i G_i\mathscr{D}_d(z_i). \tag{35}$$

In this case, $\tilde{\rho}_0(t)$ is given by

$$\tilde{\rho}_0(t) = e^{-i\tilde{\theta}t}U^{-1}P_d\mathring{\pi}U\rho, \tag{36}$$

where $\mathring{\pi}$ is the sum of the eigenprojection operators of L_d corresponding to the eigenvalues $z_i, i = 1,...,N$, i.e.,

$$\mathring{\pi} = \sum_i \pi_{z_i}, \tag{37}$$

$$\pi_{z_i} = [\mathscr{C}_d(z_i) + P_d]A_i[P_d + \mathscr{D}_d(z_i)]. \tag{38}$$

One can see from (35) that $\mathring{\pi}$ has the following expression:

$$\mathring{\pi} = [C + P_d] A [P_d + D], \tag{39}$$

$$C = \sum_i \mathscr{C}_d(z_i) F_i. \tag{40}$$

This method allows calculation of the contribution of the poles $(z_1,...,z_n)$ to the mean value $\mathrm{Tr}(O\rho(t))$ for an observable O in $\mathscr{D}(\overline{U})$. Let us denote this contribution $\langle O(t)\rangle^{\sim}$. It follows that

$$\langle O(t)\rangle^{\sim} = \mathrm{Tr}((\overline{U}O)\cdot(\Sigma(t)U\rho)),$$

where $\Sigma(t)$ is the semigroup defined in $\mathring{\pi}\mathscr{L}$ by

$$\Sigma(t) = [C + P_d] e^{-i\theta t} A [P_d + D].$$

A question arises then as to whether it is possible to find a semigroup $\widetilde{\Sigma}(t) = U^{-1}\Sigma(t)U$ in a subspace of $\mathscr{L}$ which is the range of some projector, $\tilde{\pi} = U^{-1}\mathring{\pi}U$, obtained from $\mathring{\pi}$ by similarity. This cannot be the case in our framework.[4] The mathematical reason is that the range of $\mathring{\pi}U$ cannot be included in $R(U)$. This means that the range of $\tilde{\pi}$ goes out of the space and cannot be a projection operator. To see this, let us consider some ρ in $\mathscr{D}(U)$ such that $\pi_{z_i}U\rho \in \mathscr{D}(U^{-1})$. Then, we have

$$\begin{aligned} U(L-z)^{-1}U^{-1}\pi_{z_i}U\rho &= (L_d - z)^{-1}\pi_{z_i}U\rho \\ &= -(z - z_i)^{-1}\pi_{z_i}U\rho. \end{aligned}$$

Thus,

$$(L-z)^{-1}U^{-1}\pi_{z_i}U\rho = -(z-z_i)^{-1}U^{-1}\pi_{z_i}U\rho,$$

and z_i is an eigenvalue of L, but L is a self-adjoint operator. This fact does not depend on the order of the pole z_i; it holds even when z_i is an isolated essential singularity of L_d.

Comparing with (38) our remark implies that $R(\mathscr{C}_d(z_i))$ cannot be included in $R(U)$ for $\mathrm{Im}(z_i)\neq 0$, that is what we assert in the part I concerning the impossibility of continuing analytically $\mathscr{C}(z)$ in $\rho(Q_d L_d Q_d)$ as a family of bounded operators, simultaneously with $\Psi(z)$ and $\mathscr{D}(z)Q\rho$.

We can conclude that for each initial state $\rho(0)$ belonging to the domain of the operator U, we associate a modified initial state $\tilde{\rho}(0)$ belonging to the subspace $\mathscr{F}$, $\tilde{\rho}(0) = [\widetilde{A} + \widetilde{B}]\rho(0)$, which at time t obeys an independent equation (28) in $\widetilde{\mathscr{F}}$ which is integrated by a semi-group generated by a *not necessarily* self-adjoint operator $\tilde{\theta}$.

Let us close this paragraph with some remarks on the asymptotic limit of $\tilde{\rho}_0(t)$ when $t \to +\infty$. We have to answer the following question:

$$\text{Does } \lim_{t\to\infty}\tilde{\rho}_0(t) = \lim_{t\to\infty} P\rho(t) \left(\text{or } = \lim_{T\to\infty}\frac{1}{T}\int_0^T P\rho(t)\,dt\right)?$$

As is well known, the second limit is equal to $\lim_{z\to 0^+} z P(L-z)^{-1}\rho = PE_0\rho$, where E_0 is the projection on the null space of L. In the basic works on the subdynamics theory, it was assumed that $\Psi(z)$ and $\mathscr{D}(z)$ can be analytically continued in the origin which is, furthermore, an isolated singularity of $(\Psi^{\dagger}(z) - z)^{-1}$. In this case, the contribution of the origin gives a stationary state which can exhibit the properties of equilibrium (collisional invariants) [an invariant ϕ is a collisional invariant if it satisfies $\Psi(+iO)P\phi = 0$ (see references and properties in Ref. 5]. The problem of finding a spectral deformation operator L_d, such that $[L_d - z]^{-1}$ has isolated singularity in the origin, is open. One can avoid this difficulty if the origin belongs to $\rho(Q_d L_d Q_d)$, thus $\Psi(z)$ and $\mathscr{D}(z)Q\rho$ have analytic continuations at the origin. We have the following properties:

(1) If the origin is in $\rho(Q_d L_d Q_d)$, then $E_0\rho$ is a collisional invariant for all ρ in $\mathscr{D}(U)$, i.e., $\Psi^{\dagger}(i0)E_0\rho = 0$.

Proof: If $O\in\rho(Q_d L_d Q_d)$, then $\langle Q\rho',(QLQ-z)^{-1}Q\rho\rangle$ can be analytically continued at the origin for all $\rho\in\mathscr{D}(U)$ and $\rho'\in\mathscr{D}(\overline{U})$. Then we have

$$\lim_{z\to 0^+} z\langle\rho',(QLQ-z)^{-1}Q\rho\rangle = 0.$$

On the other hand, the strong limit

$$-\lim_{z\to 0^+} z(QLQ-z)^{-1}Q = Q_0$$

exists and is equal to the projection on $N(QLQ)$. By the density of $\mathscr{D}(\overline{U})$ we have

$$\lim_{z\to 0^+} z(QLQ-z)^{-1}Q\rho = 0, \quad \rho\in\mathscr{D}(U).$$

This implies (Ref. 5), that $E_0\rho$ is a collisional invariant. (Note that in this case $\Psi^{\dagger}(i0) = U^{-1}\Psi_d(0)U$).

(2) If an element ρ in $\mathscr{D}(U)$ is such that

$$-\lim_{z\to 0^+} z(L_d - z)^{-1}U\rho = \pi_0 U\rho,$$

where π_0 is the projection operator on $N(L_d)$, then $E_0\rho\in\mathscr{D}(U)$ and

$$UE_0\rho = \pi_0 U\rho.$$

Proof: From the definition of a spectral deformation operator we have for all $\rho'\in\mathscr{D}(U^*)$, $\langle\rho',U(L-z)^{-1}\rho\rangle = \langle\rho',(L_d-z)^{-1}U\rho\rangle$, then, from our hypothesis we have

$$\langle U^*\rho',E_0\rho\rangle = \langle\rho',\pi_0 U\rho\rangle.$$

This implies that $E_0\rho\in\mathscr{D}(U)$. Q.E.D. Let us consider now the case where L_d has the following property:

$$-\lim_{z\to 0^+} z(L_d - z)^{-1}\rho = \pi_0, \tag{41}$$

where π_0 is the projection operator onto the null space of L_d. We include in $\tilde{\rho}_0(t)$ the contribution $\tilde{\rho}_0(\infty) = U^{-1}P_d\pi_0 U\rho$. By using the decomposition of $(L_d - z)^{-1}$ via P_d and Q_d and (41), we see that

$$\tilde{\rho}_0(\infty) = U^{-1}A_0[P_d + \mathscr{D}_d(0)]U\rho, \tag{42}$$

where $A_0 = P_d\pi_0 P_d$. From property (2) above we have for all $\rho\in\mathscr{D}(U)$,

$$\tilde{\rho}_0(\infty) = PE_0\rho = \lim_{T\to\infty}\frac{1}{T}\int_0^T P\rho(t)\,dt. \tag{43}$$

Finally, the null space of the operator θ is the subspace $R(A_0) = R(P_d\pi_0 P_d)$. One can easily verify (similarly to theorem III, Ref. 5) that $N(\theta) = N(\Psi_d(+iO))$ which is equivalent to $N(\tilde{\theta}) = N(\Psi(+iO))$, where $N(\tilde{\theta}) = U^{-1}R(A_0)$. This implies, by the Lagrange's multiplies theorem, that there exists an operator Ω such that

$$\tilde{\theta} = \Omega\Psi(+iO). \tag{44}$$

So we have the following result:

Theorem 1: Let ρ belong to $\mathscr{D}(U)$. If the origin belongs to $\rho(Q_d L_d Q_d)$ and if $-\lim_{z\to 0^+} z(L_d - z)^{-1} = \pi_0$, then

(1) $\lim_{t\to\infty} \tilde{\rho}_0(t) = \tilde{\rho}_0(\infty) = PE_0\rho$ and this limit is a collision invariant.

(2) $N(\tilde{\theta}) = N(\Psi(+iO))$ and there exists a linear operator Ω such that $\tilde{\theta} = \Omega\Psi(+iO)$.

Remarks: We see that the operator $U^{-1}\pi_0 U$ is well defined and $U^{-1}\pi_0 U\rho = E_0\rho$, while $U^{-1}\pi_z U$ cannot be defined when $\mathrm{Im}(z) < 0$. So we cannot derive for the correlation $Q\rho(t)$ an equation of the form

$$\tilde{\rho}_c(t) = Q\tilde{\rho}(t) = \tilde{C}\tilde{\rho}_0(t), \tag{45}$$

because $\tilde{C}$ is not defined as an operator. However, (45) can be verified for a class of observables in a weaker form:

$$\mathrm{Tr}(OQ\tilde{\rho}(t)) = \langle \bar{U}O, CU\tilde{\rho}_0(t)\rangle,$$

where $O\in\mathscr{D}(\bar{U})$ and

$$C = \sum_i \mathscr{C}_d(z_i)F_i. \tag{46}$$

In the theory of subdynamics the whole space on which L acts is decomposed into two orthogonal subspaces $\tilde{\pi}\mathscr{L}$ and $\hat{\pi}\mathscr{L}$ where $\tilde{\pi}$ and $\hat{\pi}$ are two complementary projectors. The first one is interpreted as the asymptotic part of the dynamical evolution describing the approach to equilibrium, and the second describing the transcient effects. It appears here that $\tilde{\pi}$ goes outside the space $\mathscr{L}$ and then one cannot speak of projection in the rigorous sense. In the framework of the space $\mathscr{L}$, the above decomposition can be established mathematically in $R(U)$ and understood in $\mathscr{L}$ for a class of initial states and a class of observables. Similarly, one can only define matrix elements of $\tilde{\pi}$ which cannot be considered as a proper operator in $\mathscr{L}$.

3. APPLICATION TO THE LEE MODEL

We will give an application of the preceding theory in the sector of one particle V of the Lee model without recoil effect.[6] The Hilbert space $\mathscr{H}$ is

$$\mathscr{H} = \mathscr{H}_v \oplus \mathscr{H}_{N,\theta},$$

where $\mathscr{H}_v$ is the Hilbert space of one particle V and $\mathscr{H}_{N,\theta}$ the Hilbert space of one particle N and one particle θ. A vector Ψ in $\mathscr{H}$ is given by

$$\Psi = \{a(\bar{p}), b(\bar{q},\bar{k})\},$$

$a(\bar{p})$ being a square integrable function describing a state of particle V with momentum $\bar{p} = \{p_1,p_2,p_3\}$ and $b(\bar{q},\bar{k})$ being a square integrable function describing a state of one particle N with momentum $\bar{q} = \{q_1,q_2,q_3\}$ and one particle θ with momentum $\bar{k} = \{k_1,k_2,k_3\}$. M, m, and μ will denote the mass of V, N, and θ respectively. The dynamics are described by the Hamiltonian H composed of a free part H_0 and an interaction $\lambda H_I(f)$, where λ is the coupling constant and f is a real cut-off function depending on $(\bar{p},\bar{q},\bar{k})$. We suppose further that f is a square-integrable function, i.e.,

$$\int |f(\bar{p},\bar{q},\bar{k})|^2\, d^3p\, d^3q\, d^3k < +\infty.$$

The free Hamiltonian H_0 is defined by

$$H_0\Psi = \{Ma(\bar{p}), (m + E_\theta(K))b(\bar{q},\bar{k})\}$$

for all $\Psi\in H$ such that $E_\theta(k)b(\bar{q},\bar{k})$ is square-integrable, where $E_\theta(k) = (k^2 + p^2)^{1/2}$ and $k^2 = k_1^2 + k_2^2 + k_3^2$. H_I is given by

$$H_I(f)\Psi = \left\{\int f(\bar{p},\bar{q},\bar{k})b(\bar{q},\bar{k})\,d^3p\,d^3k, \int f(\bar{p},\bar{q},\bar{k})a(\bar{p})\,d^3p\right\}.$$

$H_I(f)$ is a bounded operator of type Hilbert–Schmidt and $\mathscr{D}(H) = \mathscr{D}(H_0)$.

We introduce now the unitary representation of the dilatations group on $L^2(\mathbb{R}^n)$, $V(\gamma)$, defined by

$$(V(\gamma)f)(\bar{p}) = e^{-n\gamma/2}f(e^{-\gamma}\bar{p}).$$

for $\bar{p}\in\mathbb{R}^n$ and $\gamma\in\mathbb{R}$. Then for $\Psi\in H$, the representation of the dilations group is defined by

$$V(\gamma)\Psi = \Psi(\gamma) = \{e^{-3\gamma/2}a(e^{-\gamma}\bar{p}), e^{-3\gamma}b(e^{-\gamma}\bar{q}, e^{-\gamma}\bar{k})\}.$$

Let $\mathscr{D}(V_\beta)$ [resp. $\mathscr{D}(\bar{V}_\beta)$] be the set of vectors Ψ of $\mathscr{H}$ such that $\Psi(\gamma)$ has an analytic continuation in the strip S_β^+ (resp. S_β^-) of the complex plane, where S_β^+ (resp. S_β^-) is the strip

$$S_\beta^+ = \{\gamma\in\mathbb{C}\,|\,0\leqslant\mathrm{Im}(\gamma)\leqslant\beta<\pi/2\}$$

(respectively $S_\beta^- = \{\gamma\in\mathbb{C}\,|\,-\pi/2 < -\beta\leqslant\mathrm{Im}(\gamma)\leqslant 0\}$)

and $S_\beta = S_\beta^+ U S_\beta^-$.

We define V_β (resp. $\bar{V}_\beta$) on $\mathscr{D}(V_\beta)$ [resp. $\mathscr{D}(\bar{V}_\beta)$] by

$$V_\beta\Psi = \Psi(i\beta),$$
$$\bar{V}_\beta\Psi = \Psi(-i\beta).$$

We will suppose from now on the $f(\bar{p},\bar{q},\bar{k})$ is a *dilatation analytic cut-off function*, i.e., the family of real square-integrable functions

$$(V(\gamma)f)(\bar{p},\bar{q},\bar{k}) = E^{-\gamma 9/2}f(e^{\gamma}\bar{p}, e^{-\gamma}\bar{q}, e^{-\gamma}\bar{k})$$

can be extended to an analytic family in S_β of square-integrable functions. Then the family of operators

$$H(\gamma) = V(\gamma)HV(-\gamma)$$
$$= H_0(\gamma) + H_I(f(\gamma))$$

extends to a self-adjoint analytic family for $\gamma\in S_\beta$ [i.e., $H(\gamma)^* = H(\bar{\gamma})$] with $\mathscr{D}(H(\gamma))$ equal to the domain of H_0. This result was proved by Weder.[7]

Now the operators V_β and $\bar{V}_\beta$ are invertible self-adjoint operators and $\bar{V}_\beta = V_\beta^{-1}$ (Appendix A). Moreover, the function $\gamma\in S_\beta^+ \to \langle\varphi(\bar{\gamma}), \Psi(\gamma)\rangle$ for $\Psi,\varphi\in\mathscr{D}(V_\beta)\times\mathscr{D}(\bar{V}_\beta)$ is analytic in S_β^+ and coincides with $\langle\varphi, \Psi\rangle$ for $\gamma\in\mathbb{R}$; then

$$\langle\bar{V}_\beta\varphi, V_\beta\Psi\rangle = \langle\varphi, \Psi\rangle.$$

We shall give the application of the formalism developed above. The operator $-iH(i\beta)$, $0\leqslant\beta<\pi/2$, is a infinitesimal generator of a strongly continuous semigroup. In fact, the spectrum of $iH_0(i\beta)$ is in the first quarter of the complex plane (see Fig. 1 and Ref. 7), and as $iH_0(i\beta)$ is a normal operator, so it is an m-accretive operator (Ref. 8, p. 279) and then $-iH_0(i\beta)$ is an infinitesimal generator of a semigroup of contraction (Ref. 8, p. 485). This implies that $-iH(i\beta)$ $= -i(H_0(i\beta) + \lambda H_I(f(i\beta))$ is an infinitesimal generator on a

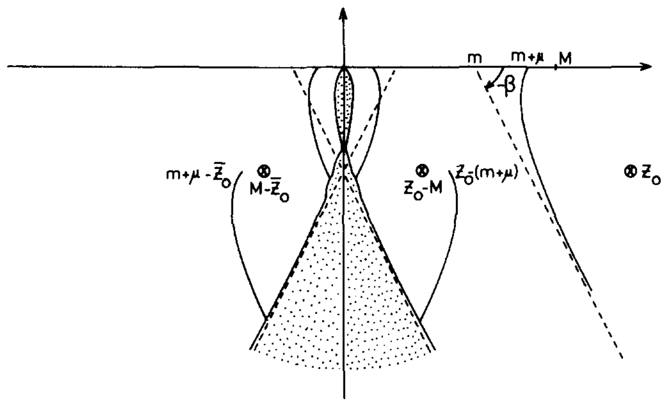

FIG. 1. The spectra of L_β and $H(i\beta)$ for $\pi/4<\beta<\pi/2$. The spectrum of $H(i\beta)$ is situated at the right of the figure while spectrum of L_β is drawn in the center.

strongly continuous semigroup of bounded operators on $\mathscr{H}$ of type $\omega_0=\lambda\,\|H_I(f(i\beta))\|$, [$H_I(f(i\beta))$ is a compact operator], by Theorem 2.1. of Chap. X of Ref. 8. Finally by the results of Aguilar, Combes, Balslev, and Weder (see, e.g., Ref. 7) $[H(\gamma)-z]^{-1}$ is analytic in S_β for Im (z) >0. This means that

$$(H-z)^{-1}\mathscr{D}\,(V_\beta)\subseteq\mathscr{D}(V_\beta)$$

and

$$V_\beta(\mathrm{H}-\mathrm{z})^{-1}\Psi=(H(i\beta)-z)^{-1}\Psi(i\beta)$$

for $\Psi\in\mathscr{D}(V_\beta)$ and $\mathrm{Im}(z)>\omega_0$. If follows that $H(i\beta)$ is a spectral deformation of H.

We introduce now the operators U'_β and $\overline{U}'_\beta$ defined on the linear spans of $\{|\varphi\rangle\langle\Psi|,\varphi,\Psi\in\mathscr{D}(V_\beta)\}$ and $\{|\varphi'\rangle\langle\Psi'|,\varphi',\Psi'\in\mathscr{D}(\overline{V}_\beta)\}$ respectively, as in Chap. 2 of I, and we take the closure of U'_β and $\overline{U}'_\beta$ which we denote by U_β and $\overline{U}_\beta$ respectively. Then, the operator L_β,

$$L_\beta\rho=[H(i\beta)\rho-\rho H(i\beta)]^{\sim},\quad\rho\in\mathscr{D}(L_\beta)$$

is a spectral deformation of L (we used the property $H(\gamma)^*=H(\overline{\gamma})$).

Theorem 2: The operators U_β and $\overline{U}_\beta$ have the following properties

(1) U_β and $\overline{U}_\beta$ are self-adjoint operators and $\overline{U}_\beta=U_\beta^{-1}$.

(2) the following two conditions are equivalent:

(i) $\rho\in\mathscr{D}(U_\beta)$.

(ii) $R(\rho)\subseteq\mathscr{D}(V_\beta)$ and $V_\beta\rho V_\beta$ extends to a Hilbert–Schmidt operator.

In this case we have $U\rho=(V_\beta\rho V_\beta)^{\sim}$.

(3) $\rho\in\mathscr{D}(U_\beta)$ if and only if $\rho^*\in\mathscr{D}(U_\beta)$ and $U_\beta\rho^*=(U_\beta\rho)^*$.

A similar theorem holds for $\overline{U}_\beta$. We give the proof in the Appendix B.

We have now to investigate the spectrum of L_β. It is easy to see that $\mathscr{L}$ is isomorphic to $\mathscr{H}\,\overline{\otimes}\,\mathscr{H}$ by noticing that the Hilbert space of the operators of Hilbert–Schmidt type on $L^2(\mathbf{R}^n)$ is isomorphic to $L^2(\mathbf{R}^n\times\mathbf{R}^n)$, which is again isomorphic to $L^2(\mathbf{R}^n)\,\overline{\otimes}\,L^2(\mathbf{R}^n)$. Furthermore, one can verify that L_β is unitarily equivalent to the closed operator $[H(i\beta)\otimes I-I\otimes H(-i\beta)]^{\sim}$. The spectrum of L_β can be deduced from the Ichinose lemma on the spectrum of a product of unbounded operators which says that $\sigma((A\otimes I-I\otimes B)^{\sim})=\sigma(A)-\sigma(\beta)$ if A and B are closed densely defined operators such that

$$\sigma(A)\subseteq\{z\in\mathbb{C}\,|\,|\arg(z)|<\theta_A\},$$
$$\sigma(B)\subseteq\{z\in\mathbb{C}\,|\,|\arg(z)|<\theta_\beta\},\quad\theta_A+\theta_B<\pi,$$

and

$$\|(A\,(\text{resp.}B)-re^{i\phi})^{-1}\|\leqslant C(\phi)/r,\quad|\phi|>\theta_A(\text{resp. }\theta_\beta).$$

So, taking $A=H(i\beta)-\lambda_0+1$ and $B=H(-i\beta)-\lambda_0+1$, where λ_0 is the minimum of the spectrum of H, the conditions of the Ichinose lemma are satisfied, the last inequality, i.e.,

$$\|(H(\pm i\beta)-\lambda_0+1-re^{i\phi})^{-1}\|\leqslant C(\phi)/r,\quad|\phi|>\beta,$$

being proved by Blaslev and Combes.[9] Then,

$$\begin{aligned}&\sigma([H(i\beta)+I-\lambda_0)\otimes I-I\otimes(H(-i\beta)-\lambda_0+I)]^{\sim})\\&=\sigma([H(i\beta)\otimes I-I\oplus H(-i\beta)]^{\sim})\\&=\sigma(H(i\beta))-\sigma(H(-i\beta))\\&=\{x-\overline{y},x,y\in\sigma(H(i\beta))\}.\end{aligned}$$

Thus we have proved the following theorem:

Theorem 3: The spectrum of L_β is the set $\{x-\overline{y},x,y\in\sigma(H(i\beta))\}$.

The operator $H(i\beta)$ was studied by Weder applying the Blaslev–Combes methods and its spectrum is known.[7]

The essential spectrum of $H(i\beta)$ is equal to the essential spectrum of $H_0(i\beta)$, it is a curve beginning in $m+\mu$ and going to infinity asymptotically to the direction $\theta=-\beta$. Each real eigenvalue of $H(i\beta)$ (different from M and $m+\mu$) is a finite-dimensional one, and it is at the same time a real eigenvalue of H. The set of those real eigenvalues is a bounded set and is independent of β. Each isolated complex eigenvalue is finite dimensional and is independent of β as long as it is not absorbed in the essential spectrum. It is finally located in the region between the curve of the essential spectrm and the real line.

It is easy to see that if $\{z_i\}$ are the eigenvalues of $H(i\beta)$, then $\{z_i-\overline{z}_j\}$ are eigenvalues of L_β. In particular, $z_i-\overline{z}_i$, whose absolute value is interpreted as the life time of the unstable V particle, is also an eigenvalue of L_β embedded in the essential spectrum of L_β. This essential spectrum is the difference between the essential spectrum of L_β and its conjugate. It contains, further, the curves beginning at $\mathrm{m}+\mu-\overline{z}_i$ and $z_i-m-\mu$, and going to the infinity in the directions $\theta=-\beta$ and $\theta=+\beta$ in the lower half-plane (see Fig.1 and Fig. 2).

We will give examples of projection P satisfying the conditions of the Sec. 3 of I.

Let $\mathscr{F}_N=\{\mathrm{a}_1(\overline{p}),...,a_N(\overline{p})\}$ be a finite orthonormal family of $\mathscr{H}_V$, and such that $V(\gamma)a_i$ extends to an analytic family of vectors of $\mathscr{H}_V$ *for* $\gamma\in S_\beta$. Then the projector P_N given by

$$P_N\rho=\sum_{n=1}^{N}\langle a_n,\rho a_n\rangle|a_n\rangle\langle a_n|,$$

which projects on a subspace of N($[H_0,\cdot]$) fulfills all the requirements formulated in I. The projection operator $P_{N,\beta}$ is

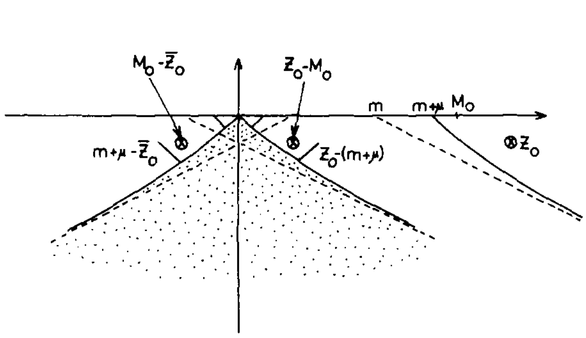

FIG. 2. This figure represents the spectra of L_β and $H(i\beta)$ for $0<\beta\leqslant\pi/4$ similarly as in the Fig. 2.

given by

$$P_{N,\beta}\rho = \sum_n |\rho_{n,\beta}\rangle\langle\rho_{n,\beta}|,$$

where $\rho_{n,B} = |a_n(i\beta)\rangle\langle a_n(i\beta)|$. If furthermore P_N converges strongly to P, then $P = \lim_{N\to\infty} P_N$ fulfills the same requirements, as can be easily verified. This convergence occurs if, for example, the orthonormal system $\{a_n\}$ satisfies $\sum\|a_n(\pm i\beta)\|^2 < +\infty$. Then, one easily verifies that

(i) $R(P)\subset\mathscr{D}(U_\beta)\cap\mathscr{D}(\bar{U}_\beta)\cap\mathscr{D}(L)$,

(ii) $R(P_\beta)\subset N(L_{O,\beta})\subset\mathscr{D}(L_\beta)$,

(iii) $R(P^*_\beta)\subset N(L^*_{O,\beta})\subset\mathscr{D}(L^*_\beta)$,

for $L^*_{O,\beta} = L_{O,-\beta}$ and $L_{O,\beta}|a\rangle\langle a'| = 0$ when $|\beta|<\pi/2$ and $a,a'\in\mathscr{H}_V$. Here L_0 denotes $[H_0,\cdot]$.

We have now to investigate the extended domain of analyticity of $\Psi(z)$, $\mathscr{D}(z)Q\rho$, and $[\Psi(z)-z]^{-1}$, that is the intersection of the lower half-plane with $\rho(Q_\beta L_\beta Q_\beta)$. The essential spectrum of $Q_\beta L_\beta Q_\beta$ is the limit of the domain of analyticity of $\Psi^\dagger(z)$, etc. Let us characterize this essential spectrum for finite-dimensional projection operator P.

As P_β is finite-dimenensional projection operator, it is then compact, and so is $P_\beta\delta L_\beta$ and $\delta L_\beta P_\beta$, where δL_β denotes the commutator $[H_I(f(i\beta)),\cdot]$. Let $y_0>\alpha_0+\|\delta L_\beta P_\beta - P_\beta\delta L_\beta\|$. Then

$$\|\delta L_\beta P_\beta - \delta L_\beta P_\beta(L_\beta - iy)^{-1}\|\leqslant 1, \tag{47}$$

where α_0 is the type of the semigroup generated by $-iL_\beta$. Equation (47) is a consequence of the following inequality (Ref. 8, p. 485):

$$\|1/(L_\beta - iy)\| < 1/(y-\alpha_0) \quad \text{for } y>\alpha_0.$$

The condition (47) is sufficient to prove that the essential spectrum of $Q_d L_d Q_d$ is equal to the essential spectrum of L_β.[8]

CONCLUSIONS

We have studied the possibility of a construction of the theory of subdynamics which describes the irreversible phenomena in the frame of the space of Hilbert–Schmidt operators. We have tried to investigate conditions under which different steps of the formal construction could be realized in this frame.

Firstly, the problem of the existence of analytic continuation of matrix elements of the resolvent of the Liouville–von Neumann operator can be solved under some conditions. Such a condition is the existence of a spectral deformation of L by a non-self-adjoint operator for which the essential spectrum lies in the lower half-plane. This condition can be verified in the Lee model when the interaction has some analyticity properties; this is an application of the Combes–Blaslev theory. The class of matric elements of the resolvent of Liousville–von Neumann operator admitting analytic continuation is characterized by the domains of two unbounded operators, and these domains cannot be equal to the whole space. Thus, the construction of analytic continuation is also a restriction to a class of initial states having some regularity properties.

Secondly, the study of the contributions of poles which are solutions of a dispersion relation is possible for some choices of the projection operator P, and consequently, of the representation which defines diagonal elements. Such conditions are related to a domain of regular diagonal matrices density having the above analyticity properties. In this case, it is possible to show that some contribution $\tilde{\rho}_0(t)$ of the diagonal part $\rho_0(t)$, obeys an evolution generated by a non-Hermitian operator $\tilde{\theta}$ and this contribution tends to a collisional invariant when the initial state has some analyticity properties.

However, here we cannot speak about a subdynamics in the proper sense of a closed subspace in which e^{-itL} reduces to a semigroup for $t>0$ and which is the range of a projection operator $\tilde{\pi}$. In this frame we may only define matrix elements of the so-called $\tilde{\pi}$ operator. The passage from these matrix elements to a proper operator requires supplementary mathematical structure and this goes beyond the frame of the Hilbert–Schmidt operators considered here.

APPENDIX A

The operator V_β and $\bar{V}_\beta$ (defined in Sec. 3) are invertible self-adjoint operators and $\bar{V}_\beta = V_\beta^{-1}$.

Proof: If $V(\gamma)\Psi = \Psi(\gamma)$ is analytic in S^+_β, then for $\gamma\in S^+_\beta$ and $\alpha\in\mathbb{R}$, $V(\alpha)\Psi(\alpha) = \Psi(\gamma+\alpha)$. Thus, $V(\gamma)\Psi(i\beta) = \Psi(\gamma+i\beta)$ for all $\gamma\in\mathbb{R}$ and it is analytic in S^-_β. This means that $\Psi(i\beta)\in\mathscr{D}(\bar{V}_\beta)$ and $\bar{V}_\beta\Psi(i\beta) = \Psi$. By inverting V_β and $\bar{V}_\beta$ we prove that $V_\beta\bar{V}_\beta\subset\mathbb{1}$, and the last assertion follows. Let up prove the self-adjointness. For all Ψ, $\Psi'\in\mathscr{D}(V_\beta)$, the functions $\langle\Psi',\Psi(\gamma)\rangle$ and $\langle\Psi'(-\bar{\gamma}),\Psi\rangle$ are analytic in S^+_β, and for $\gamma\in\mathbb{R}$, $\langle\Psi',\Psi(\gamma)\rangle = \langle\Psi'(-\gamma),\Psi\rangle$. By the uniqueness of the analytic continuation we have

$$\langle\Psi',\Psi(i\beta)\rangle = \langle\Psi'(i\beta),\Psi\rangle,$$

thus $V_\beta\subset V^*_\beta$. Let, $\Psi\in\mathscr{D}(V^*_\beta)$, then for all $\varphi\in\mathscr{D}(V_\beta)$, $\langle\varphi,\Psi(-\gamma)\rangle = \langle\varphi(\gamma),\Psi\rangle$, $\gamma\in\mathbb{R}$, has an analytic continuation $\langle\varphi(\bar{\gamma}),\Psi\rangle$ in S^-_β. If we prove that $\langle\varphi,\Psi(-\gamma)\rangle$ has an analytic continuation in S^-_β for all $\varphi\in\mathscr{H}$, then $\Psi(\gamma)$ has an analytic continuation in S^+_β, that is $\psi\in\mathscr{D}(V_\beta)$.

By the density of the domain of V_β, there exists a sequence $\varphi_n\in\mathscr{D}(V)$ such that $\varphi_n\to\varphi$ for all $\varphi\in\mathscr{H}$. $\langle\varphi_n(\bar{\gamma}),\Psi\rangle,\gamma\in S^-_\beta$ is a sequence of analytic functions which converges for $\gamma\in\mathbb{R}$ to $\langle\varphi(\gamma),\Psi\rangle = \langle\varphi,\Psi(-\gamma)\rangle$. This sequence is uniformly bounded for $\gamma\in\mathbb{R}$ and for all

$\gamma = \alpha + i\beta$. In fact

$$|\langle \varphi_n(\alpha + i\beta), \Psi\rangle| = |\langle V_\beta V(\alpha)\varphi_n, \Psi\rangle| = |\langle \varphi_n(\alpha), V_\beta^* \Psi\rangle| \leqslant \|\varphi_n\| \|V_\beta^* \Psi\| \leqslant M \|V_\beta^* \Psi\|.$$

Then, $\langle \varphi_n(\bar\gamma), \Psi\rangle$ is bounded in S_β^- and it converges by Vitali's theorem to an analytic function in S_β^-, and we have

$$\lim_{n\to\infty} \langle \varphi_n(\gamma), \Psi\rangle = \langle \varphi, \Psi(-\gamma)\rangle, \quad \gamma \in S_\beta^-$$

$$\langle \varphi, \Psi(i\beta)\rangle = \lim_{n\to\infty} \langle \varphi_n(i\beta), \Psi\rangle = \lim_{n\to\infty} \langle \varphi_n V_\beta^* \Psi\rangle = \langle \varphi, V_\beta^* \Psi\rangle,$$

i.e., $V_\beta^* \Psi = \Psi(i\beta) = V_\beta \Psi$.

APPENDIX B

Proof of Theorem 2: We will prove first that if A and B are self-adjoint operators in $\mathscr{H}$, then the closure of the operator $A \times B$ defined on the linear span of $\{|\varphi\rangle\langle\Psi|, \varphi \in \mathscr{D}(A), \Psi \in \mathscr{D}(B)\}$ by $(A \times B)|\varphi\rangle\langle\Psi| = |A\varphi\rangle\langle B\Psi|$ is self-adjoint. One can easily verify that $A^* \times B^* = A \times B \subset (A \times B)^*$. Then $A \times B$ is symmetric. Let $E(\Delta)$ and $F(\Delta)$ be the spectral families of A and B corresponding to the finite Borel set $\Delta \subset \mathbb{R}$. The union of $\{E(\Delta)\Psi, \Psi \in \mathscr{H}, \Delta \subset \mathbb{R}\}$ is dense in $\mathscr{H}$, and similarly for $F(\Delta)$. Then the linear span of $\{|E(\Delta)\varphi\rangle\langle F(\Delta')\Psi|, \varphi, \Psi \in \mathscr{H}\}$ is a dense set in $\mathscr{L}$ of analytic vectors for $A \times B$; this follows from

$$\sum \| |A^n E(\Delta)\varphi\rangle\langle B^n F(\Delta')\Psi| \| t^n/n! = \sum \|A^n E(\Delta)\varphi\| \|B^n F(\Delta')\varphi\| t^n/n! \leqslant e^{\|AE(\Delta)\| \|BF(\Delta')\| t} \|\varphi\| \|\Psi\|,$$

and by the Nelson Lemma $A \times B$ is essentially self-adjoint. This proves the self-adjointness of U_β and $\bar U_\beta . \bar U_\beta = \bar U_\beta^{-1}$ is evident, and the second part follows from Appendix B of I. Let $\rho \in \mathscr{D}(U_\beta)$, then for $\varphi, \Psi \in \mathscr{D}(V_\beta)$ we have

$$\langle V_\beta \rho V_\beta \Psi, \varphi\rangle = \langle V_\beta \Psi, \rho^* V_\beta \varphi\rangle = \langle \Psi, (V_\beta \rho V_\beta)^* \varphi\rangle;$$

thus $\rho^* V_\beta \varphi \in \mathscr{D}(V_\beta)$ and $V_\beta \rho^* V_\beta \subset (V_\beta \rho V_\beta)^*$. This implies that $\rho^* \in \mathscr{D}(U_\beta)$ and $U_\beta \rho^* = (U_\beta \rho)^*$. The proof of the theorem is complete.

This theorem characterizes completely $\mathscr{D}(U_\beta)$. It is known that the Hilbert space of the operators of Hilbert–Schmidt class of $L^2(\mathbb{R}^n)$ is isomorphic to $L^2(\mathbb{R}^n \times \mathbb{R}^n)$. Then for all $\rho \in \mathscr{L}$ there exists four kernels $\rho_{V,V}(\bar p, \bar p')$, $\rho^{V,N\theta}(\bar p, \bar q', \bar k')$, $\rho_{N\theta,V}(\bar q, \bar k, \bar p')$, $\rho_{N\theta,N\theta}(\bar Q, \bar k, \bar q', \bar k)$ such that

$$\rho\Psi = \Big\{ \int \rho_{V,V}(p, \bar p') a(\bar p')\, d^3p' + \int \rho_{V,N\theta}(\bar p, \bar q', \bar k') b(\bar q', \bar k')\, d^3q'\, d^3k',$$
$$\int \rho_{N\theta,V}(\bar q \bar k, \bar p') \alpha(\beta')\, d^3p' + \int \rho_{N\theta,N\theta}(\bar q, \bar k, \bar q', \bar k') b(\bar q', \bar k')\, d^3q'\, d^3k' \Big\}$$

for all given $\Psi = \{a(\bar p'), b(\bar q', \bar k')\}$.

Corollary: The following two conditions are equivalent for all $\rho \in \mathscr{L}$:

(1) $\rho \in \mathscr{D}(U_\beta)$,

(2) The family of operators $\rho_{\gamma,\gamma'} = V(\gamma)\rho V(\gamma')$, $\gamma, \gamma' \in \mathbb{R}$, has the following property:

(i) $\rho_{\gamma\gamma_0'}$ (resp. $\rho_{\gamma_0,\gamma'}$) extends to an analytic family of bounded operators for all $\gamma \in S_\beta^+$ and fixed $\gamma'_0 \in \mathbb{R}$ (resp. for all $\gamma' \in S_\beta^-$ and fixed $\gamma_0 \in \mathbb{R}$).

(ii) $\rho_{i\beta,\gamma'}$ (resp. $\rho_{\gamma,-i\beta}$) extends to an analytic family of bounded operators in S_β^- (resp. S_β^+).

(iii) $\rho_{i\beta,-i\beta}$ is an operator of Hilbert–Schmidt type.

In this case

$$U_\beta \rho = \rho_{i\beta,-i\beta}.$$

Proof: $1 \Rightarrow 2$. Let $\rho \in \mathscr{D}(U_\beta)$. By Theorem 2, $\rho^* \in \mathscr{D}(U_\beta)$, and for all $\Psi \in \mathscr{H}$, $V(\gamma)\rho^*\Psi$ extends to an analytic family of vectors of $\mathscr{H}$ in S_β^+. Let $V_\gamma = V(a)V_b$ for $\gamma = a + ib$. It is easy to see that $V_\gamma = V_b V(a)$. Thus $V_\gamma \rho^*$ is a bounded operator ($R(\rho^*) \subset \mathscr{D}(V_b)$) and $V_\gamma \rho^* V(-\gamma_0') = \rho^*_{\gamma,\gamma_0'}$ is an analytic family of bounded operators for all $\gamma \in S_\beta^+$. On the other hand,

$$\rho^*_{\gamma,\gamma_0'}(\bar p, \bar p') = \overline{\rho_{\gamma_0',\bar\gamma}(\bar p', \bar p)},$$

where we omit the index (v,v) from $\rho_{v,v}(\bar p, \bar p')$ for economy of notation. The other kernels of ρ have the same properties. This implies that $\rho_{\gamma_0,\gamma'}$ is an analytic family of bounded operators for all $\gamma' \in S_\beta^-$, and one sees easily that $\rho_{\gamma_0,\gamma'} = V(\gamma_0)[\rho V_{b'}]^\sim V(a')$, where $\gamma' = a' + ib' \in S_\beta^-$.

Similarly by Theorem 2, $V(\gamma)\rho V(-\gamma_0')\Psi$ extends to an analytic family of vectors of $\mathscr{H}$ in S_β^+, and $\rho_{\gamma,\gamma_0'}$ is a family of bounded operators analytic in S_β^+. This proves (i). To prove (ii) one remarks that $R([\rho V_\beta]^\sim) \subset \mathscr{D}(V_\beta)$. For if $\Psi \in \mathscr{H}$, then by the density of $\mathscr{D}(V_\beta)$ there exists a sequence $\Psi_n \in \mathscr{D}(V_\beta)$ such that $\Psi_n \to \Psi$. Thus $\rho V_\beta \Psi_n \to [\rho V_\beta]^\sim \Psi$, $n \to \infty$ and $V_\beta \rho V_\beta \Psi_n$ is convergent, and this implies that $\rho V_\beta \Psi \in \mathscr{D}(V_\beta)$. This means that $\rho_{\gamma,-i\beta}$ is again a family of bounded operators analytic in S_β^+. Similarly, $V_\gamma[\rho^* V_\beta]$ is an analytic family of bounded operators in S_β^+, and this implies that ρ is an analytic family bounded operators in S_β^-. It is evident that $\rho_{i\beta,-i\beta} = V_\beta \rho V_\beta$, and (iii) is immediate.

The converse is an easy consequence of the Theorem 2.

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Densities of covariant observables [a)]

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Positive-operator-valued observables in a complex Hilbert space $\mathfrak{H}$ based on a topological homogeneous space G/H and G-covariant with respect to a strongly continuous unitary representation on $\mathfrak{H}$ of a locally compact group G are investigated. The goal is to determine whether they are the weak integrals of some positive-operator-valued densities relative to a G-quasi-invariant measure μ on G/H. To this end, the notion of a kernel Hilbert space is generalized to spaces of equivalence classes with respect to μ of mappings of G/H into a complex Hilbert space $\mathfrak{K}$.

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I. INTRODUCTION

The notion of an observable introduced by Davies and Lewis[1] in their axiomatic approach to statistical physical theories differs from the usual one in two respects. In the first place, the space of which an observable is based is not always a subset of **R** and, secondly, an observable is not necessarily a projection-valued measure on a subset of **R** (or, what amounts to the same by the spectral theorem, a self-adjoint (linear) operator). Davies and Lewis define an observable as a positive-operator-valued measure on a set X, equipped with a σ-field of subsets, and taking values in the topological dual space V' of a real Banach space V when V' is equipped with the weak-* topology. The physical meaning of X is either that of a configuration or of a phase space, while V is interpreted as a state space. Using this definition, a joint observable for position and momentum in phase space, which gives the probabilities of approximate simultaneous measurements, can be constructed (Ref. 2,3.4) and a position observable for the photon (a "fuzzy observable"[3]) can be exhibited (cf. also Ref. 4).

In what follows, we shall restrict ourselves to consider a real Banach space V which describes an irreducible quantum system without superselection rules, namely, the Banach space (with the trace norm) of all self-adjoint trace class operators in a complex Hilbert space $\mathfrak{H}$. Then V' is the set of all self-adjoint elements of the complex vector space $\mathscr{L}(\mathfrak{H})$ of all continuous (linear) operators in $\mathfrak{H}$. We shall suppose $\mathscr{L}(\mathfrak{H})$ endowed with the weak operator topology, since with this topology we obtain the same observables as with the ultraweak one. Moreover, our observables will be based on sets X which are locally compact spaces, and they will be G-covariant with respect to some strongly continuous unitary representations of a locally compact group G. Our goal will be the characterization of G-covariant observables, on a transitive topological G-space X, which admit a density, i.e., which are the weak integrals of a family (parametrized by X) of continuous positive operators.

In Sec. II, we recollect some basic definitions and facts concerning observables, G-covariance, etc., and introduce the notion of a density of an observable. We investigate in Sec. III a generalization of the usual concept of a kernel Hilbert space (by allowing spaces of classes of mappings), and then we establish in Sec. IV the equivalence between the existence of a density of a given covariant observable and the possibility of identifying its carrier space with a certain kernel Hilbert space.

Throughout the paper, every group operation considered will be tacitly assumed to be a *left* one; consequently, every quasi-invariant (resp. invariant) measure will be *left quasi-invariant* (resp. *left invariant*). The term "measure," with the exceptions of "POV-measure" and "PV-measure" in Sec. II, has to be understood as "real Radon measure" and measurability will always be in Bourbaki sense (Ref. 5, Chap. 4, §5). If X is a locally compact space, we shall denote by $\mathscr{B}_X$ the Borel structure (i.e., the σ-field) generated by its closed sets. The symbol ϕ_A will stand for the characteristic function of a set A, and $[f]$ for the equivalence class of a mapping f with respect to the measure in point. If $\mathfrak{K}$ is a Hilbert space, then $(\cdot|\cdot)_{\mathfrak{K}}$ (resp. $\|\cdot\|_{\mathfrak{K}}$) will denote its scalar multiplication (resp. its norm); as usual, the adjoint of a linear mapping A of Hilbert spaces will be denoted by A^*.

II. PRELIMINARIES

Let X be a locally compact space, and let $\mathfrak{H}$ be a complex Hilbert space. An *observable* in $\mathfrak{H}$ based on X is a normalized (weak) Borel positive-operator-valued measure (concisely, a Borel POV-measure) on X acting in $\mathfrak{H}$, namely, a mapping $M:\mathscr{B}_X \rightarrow \mathscr{L}(\mathfrak{H})$ satisfying the following conditions:

(i) M is positive, i.e., $M(B) \geqslant 0$ for all $B \in \mathscr{B}_X$ and $M(\varnothing) = 0$.

(ii) M is (weakly) countably additive, i.e., if $(B_i)_{i\in \mathbf{N}}$ is a sequence of mutually disjoint elements of $\mathscr{B}_X$, then

$$M\Big(\bigcup_{i=0}^{\infty} B_i\Big) = \text{w-}\sum_{i=0}^{\infty} M(B_i), \tag{II.1}$$

where "w-Σ" means convergence in the weak operator topology on $\mathscr{L}(\mathfrak{H})$.

(iii) $M(X) = \mathrm{Id}_{\mathfrak{H}}$ (normalization).

We say that M is a *decision* (or *sharp*) *observable*[6] when, in addition to (i)–(iii), the following condition is satisfied:

(iv) $M(B)M(B') = M(B\cap B')$ for all B,B' in $\mathscr{B}_X$.

In other words, a decision observable is a normalized Borel projection-valued measure (concisely, a Borel PV-measure).

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Remark 1: The convergence of (II.1) in the weak operator topology also implies convergence in the strong operator, ultraweak, and ultrastrong topologies (Ref. 7, Remark 1).

Definition 1: Let X be a locally compact space, let μ be a measure on X, and let $\mathfrak{H}$ be a complex Hilbert space. An observable M in $\mathfrak{H}$ based on X is said to *admit a μ-density* if there exists a mapping $D_M: x \mapsto M_x$ (a *μ-density*), defined $\mu(x)$-a.e. in X, and taking its values in the set $\mathscr{L}(\mathfrak{H})^+$ of all positive continuous operators in $\mathfrak{H}$, such that

$$M(B) = \int \phi_B(x) M_x d\mu(x) \quad \textit{weakly}$$

for all $B \in \mathscr{B}_X$.

Notice that the μ-density D_M is unique $\mu(x)$-a.e.

Given a locally compact group G, a locally compact G-space X, a strongly continuous unitary representation U of G on a complex Hilbert space $\mathfrak{H}$ and an observable M in $\mathfrak{H}$ based on X, we say that M is *G-covariant* with respect to U if the pair U,M satisfies

$$U(g)M(B)U(g)^{-1} = M(g \cdot B)$$

for all $g \in G$ and all $B \in \mathscr{B}_X$. The G-covariant observable M is said to be *transitive* if so is the G-space X. Two observables, M in $\mathfrak{H}$ and M' in $\mathfrak{H}'$, which are both based on X and G-covariant with respect to U and U', respectively, are said to be *unitarily equivalent* if there exists a unitary mapping V of $\mathfrak{H}$ onto $\mathfrak{H}'$ such that

$$VU(g) = U'(g)V \quad \text{for all } g \in G$$

and

$$VM(B) = M'(B)V \quad \text{for all } B \in \mathscr{B}_X.$$

Remark 2: An observable M in $\mathfrak{H}$ based on X determines a *Radon observable* M_R based on X and taking its values in $\mathscr{L}_s^w(\mathfrak{H})$, namely, in the vector space $\mathscr{L}(\mathfrak{H})$ equipped with the weak operator topology (Ref. 8, § 2). Let $\mathscr{C}_C^0(X)$ be the complex Banach space of all continuous complex-valued functions on X vanishing at infinity. Then M_R is the continuous linear mapping of $\mathscr{C}_C^0(X)$ into $\mathscr{L}_s^w(\mathfrak{H})$ defined by

$$M_R(f) = \int f(x) dM(x) \quad (f \in \mathscr{C}_C^0(X));$$

it satisfies $M_R(f) \geqslant 0$ whenever $f \geqslant 0$ and is such that

$$\|M_R(f)\| \leqslant \sup_{x \in X} |f(x)|.$$

The Radon observable M_R is G-covariant with respect to U if

$$U(g)M_R(f)U(g)^{-1} = M_R(g \cdot f) \quad (f \in \mathscr{C}_C^0(X)),$$

where $g \cdot f$ is defined by $(g \cdot f)(x) = f(g^{-1} \cdot x)$.

In the following, we shall formulate every result in terms of observables defined as POV-measures; the translation in the language of Radon observables is straightforward.

Let $G,X,\mu,\mathfrak{H}$, and U be as above and suppose in addition that μ is G-quasi-invariant. If an observable M in $\mathfrak{H}$ based on X is G-covariant with respect to U and admits a μ-density $D_M: x \mapsto M_x$, then, for each $g \in G$, we have

$$U(g)M_x U(g)^{-1} = \alpha(g,x) M_{g \cdot x} \quad \mu(x)\text{-a.e.} \tag{II.2}$$

Here α is a quasi-invariance factor of μ, i.e., a real-valued function on $G \times X$ such that, for each $g \in G$,

$$\mu_g = \alpha(g,\cdot) \cdot \mu,$$

where the measure μ_g is defined by $\mu_g(A) = \mu(g \cdot A)$ for all μ-integrable sets A.

If H is a closed subgroup of G and X is the (topological) homogeneous space G/H, there always exists a nontrivial positive G-quasi-invariant measure μ on X unique up to equivalence (Ref. 9, Chap. 7, § 2, Theorems 1 and 2), i.e., a nontrivial positive measure μ on X such that, for each $g \in G$, the measure μ_g is equivalent to μ. More precisely, let π be the canonical mapping of G onto G/H and let Δ_G (resp. Δ_H) be the modulus function of G (resp. of H). There exist continuous real-valued functions $\rho > 0$ on G satisfying

$$\rho(gh) = (\Delta_H(h)/\Delta_G(h))\rho(g)$$

for all $g \in G$ and all $h \in H$, defining a nontrivial positive G-quasi-invariant measure μ on G/H with a quasi-invariance factor α given by

$$\alpha(g,\pi(g')) = \rho(gg')/\rho(g') \tag{II.3}$$

for all g,g' in G. We shall then say that μ is *defined by a ρ-function*. Moreover, we shall denote by $\mu^{\#}$ the unique measure on G such that

$$\int_G f^{\#}(g) d\mu^{\#}(g) = \int_{G/H} d\mu(\pi(g)) \int_H f^{\#}(gh) d\nu(h)$$

for all continuous real-valued functions $f^{\#}$ on G with compact support, where ν is any Haar measure on H. Hence $\mu^{\#}$ is the measure with density ρ relative to some Haar measure on G (Ref. 9, Chap. 7, § 2, Lemmas 4 and 5).

Proposition 1: Let G be a locally compact group, let H be a closed subgroup of G, and let μ be a nontrivial positive G-quasi-invariant measure on G/H defined by a ρ-function. If M is an observable in a complex Hilbert space $\mathfrak{H}$ based on G/H, if it is G-covariant with respect to a strongly continuous unitary representation U of G on $\mathfrak{H}$, and if, in addition, it admits a μ-density $D_M: x \mapsto M_x$ such that M_x is a projection $\mu(x)$-a.e., then μ is G-invariant.

Proof: By taking the square of (II.2), we obtain, for each $g \in G$,

$$\alpha(g,x) = 1 \quad \mu(x)\text{-a.e.},$$

whence the G-invariance of μ. ■

Remark 3: If, in Proposition 1, U is irreducible and M_x is a one-dimensional projection $\mu(x)$-a.e., then M is the observable defined by a system of coherent states relative to U based on G/H (Ref. 2, 8.5, Theorem 5.2; Ref. 10).

Let G,H,π,μ be as above. We denote by $\mathrm{Ind}_H^G U$ the (strongly continuous unitary) representation of G induced by a strongly continuous unitary representation U of H on a complex Hilbert space, say $\mathfrak{K}$. We shall assume that $\mathrm{Ind}_H^G U$ is carried by $L^2_{\mathfrak{K}}(G/H,\mu;U)$, a complex Hilbert space defined as follows (cf., for instance, Ref. 11, Chap. VI, § 4, Theorem 15). Let s be an arbitrary but fixed section associated with π, and let $\mathscr{S}$ be the complex vector space of mappings of G/H into $\mathfrak{K}$ generated by all μ-negligible ones and by all those of the form $f^{\#} \circ s$, where $f^{\#}$ is a continuous mapping of G into $\mathfrak{K}$ satisfying

$$f^{\#}(gh) = U(h)^{-1} f^{\#}(g) \tag{II.4}$$

for all $g \in G$ and all $h \in H$ and such that the function $x \mapsto \|f^{\#}(s(x))\|_{\mathfrak{K}}$ on G/H has compact support. We denote by $\mathscr{L}^2_{\mathfrak{K}}(G/H,\mu;U)$ the completion of $\mathscr{S}$ in the locally convex complex vector space of all mappings f of G/H into $\mathfrak{K}$ such that the function $x \mapsto \|f(x)\|^2_{\mathfrak{K}}$ is μ-integrable on G/H and whose topology is defined by the seminorm

$$f \mapsto \left(\int \|f(x)\|^2_{\mathfrak{K}}\, d\mu(x) \right)^{1/2}.$$

If $f \in \mathscr{L}^2_{\mathfrak{K}}(G/H,\mu;U)$ is not μ-negligible, there exists a $\mu^{\#}$-measurable mapping $f^{\#}$ of G into $\mathfrak{K}$ satisfying (II.4) and $f^{\#} \circ s = f$. Notice that if a mapping $f^{\#}$ of G into $\mathfrak{K}$ satisfying (II.4) is $\mu^{\#}$-measurable, the function $g \mapsto \|f^{\#}(g)\|_{\mathfrak{K}}$ is $\mu^{\#}$-measurable on G and the function $x \mapsto \|f^{\#}(s(x))\|_{\mathfrak{K}}$ is μ-measurable on G/H (Ref. 9, Chap. 7, § 2, Proposition 6). Then $L^2_{\mathfrak{K}}(G/H,\mu;U)$ is the Hausdorff space associated with $\mathscr{L}^2_{\mathfrak{K}}(G/H,\mu;U)$. We have, for each $g \in G$,

$$(\mathrm{Ind}_H^G U)(g)[f] = [f_g] \quad (f \in \mathscr{L}^2_{\mathfrak{K}}(G/H,\mu;U)), \tag{II.5}$$

where $f_g(x) = \alpha(g^{-1},x)^{1/2} f(g^{-1}\cdot x)$ $(x \in G/H)$.

If G is second countable, there exists a Borel section associated with π and, via this section, $L^2_{\mathfrak{K}}(G/H,\mu;U)$ can be identified with $L^2_{\mathfrak{K}}(G/H,\mu)$, the complex Hilbert space of all μ-square-integrable mappings of G/H into $\mathfrak{K}$.

We shall denote by $P_{\mathfrak{K}}$ the decision observable in $L^2_{\mathfrak{K}}(G/H,\mu;U)$ based on G/H defined by

$$P_{\mathfrak{K}}(B)[f] = [\phi_B f] \quad ([f] \in L^2_{\mathfrak{K}}(G/H,\mu;U);\, B \in \mathscr{B}_{G/H}).$$

Proposition 2: Let G be a locally compact group, let H be a closed subgroup of G, let μ be a nontrivial positive G-quasi-invariant measure on G/H defined by a ρ-function, and let $\mathfrak{H}$ be a complex Hilbert space. If M is an observable in $\mathfrak{H}$ based on G/H, which is G-covariant with respect to a strongly continuous unitary representation U of G on $\mathfrak{H}$, there exist a strongly continuous unitary representation $\gamma(U)$ of H on a complex Hilbert space $\mathfrak{K}$ and an isometric mapping V of $\mathfrak{H}$ into $L^2_{\mathfrak{K}}(G/H,\mu;\gamma(U))$ satisfying

$$U(g) = V^*(\mathrm{Ind}_H^G \gamma(U))(g)V \quad \text{for all } g \in G,$$

$$M(B) = V^* P_{\mathfrak{K}}(B) V \quad \text{for all } B \in \mathscr{B}_{G/H},$$

and such that the set

$$\{P_{\mathfrak{K}}(B)V\phi \mid B \in \mathscr{B}_{G/H} \text{ and } \phi \in \mathfrak{H}\}$$

is total in $L^2_{\mathfrak{K}}(G/H,\mu;\gamma(U))$. The mapping V is surjective if and only if M is a decision observable. The triple $(L^2_{\mathfrak{K}}(G/H,\mu;\gamma(U)), \mathrm{Ind}_H^G \gamma(U), P_{\mathfrak{K}})$ is unique up to unitary equivalence.

Proof: See Ref. 7, Proposition 2 and end of Sec. 3.■

III. KERNEL HILBERT SPACES

In this section, we generalize the notion of a kernel Hilbert space from that of a space of complex-valued functions[12,13] defined in a locally compact space X to that of a space of equivalence classes with respect to some measure of mappings of X into a complex Hilbert space. Following the lines traced by Kunze[14] in the case of continuous mappings, we emphasize the relation between the existence of a kernel and the continuity of some "evaluation mappings" (cf. also Refs. 15 and 16).

Definition 2: Let X be a locally compact space, let μ be a measure on X, and let $\mathfrak{K}$ be a complex Hilbert space. A *positive μ-kernel* K on X acting in $\mathfrak{K}$ is a mapping of $X \times X$ into $\mathscr{L}(\mathfrak{K})$ satisfying

$$\sum_{j \in J, k \in J} (K(x_k,x_j)\phi_j \mid \phi_k)_{\mathfrak{K}} \geqslant 0 \tag{III.1}$$

for all finite index sets J, all x_j, x_k in X, and all ϕ_j, ϕ_k in $\mathfrak{K}$. It is said to be *admissible* if the relation $[K(\cdot,y)\phi] = [K(\cdot,z)\psi]$ between equivalence classes with respect to μ of mappings of X into $\mathfrak{K}$ implies $K(\cdot,y)\phi = K(\cdot,z)\psi$ for all y,z in X an all ϕ,ψ in $\mathfrak{K}$.

A *square-integrable positive μ-kernel* (on X acting in $\mathfrak{K}$) is a positive μ-kernel K such that the mapping $K(\cdot,y)\phi$ is μ-square-integrable for all $y \in X$ and all $\phi \in \mathfrak{K}$, satisfying in addition

$$\int (K(x,y)\phi \mid K(x,z)\psi)_{\mathfrak{K}}\, d\mu(x) = (K(z,y)\phi \mid \psi)_{\mathfrak{K}} \tag{III.2}$$

for all y,z in X and all ϕ,ψ in $\mathfrak{K}$.

Remark 4: By reason of (III.1), the operator $K(x,x)$ is positive for all $x \in X$. In addition, we have $K(x,y)^* = K(y,x)$ for all x,y in X because (III.1) and the positivity of $K(x,x)$ and $K(y,y)$ imply

$$\mathrm{Im}((K(x,y)^* - K(y,x))\phi \mid \psi)_{\mathfrak{K}} = 0$$

for all ϕ,ψ in $\mathfrak{K}$.

Let $\mathscr{F}(X;\mathfrak{K})$ be the complex vector space of all mappings of X into $\mathfrak{K}$ and let $F(X;\mathfrak{K})$ be the quotient vector space of all its equivalence classes with respect to μ. We shall call a *μ-selection* every linear mapping σ of $F(X;\mathfrak{K})$ into $\mathscr{F}(X;\mathfrak{K})$ such that $[\sigma([f])] = [f]$ for all $f \in \mathscr{F}(X;\mathfrak{K})$.

Proposition 3: Let K be an admissible positive μ-kernel on a locally compact space X, equipped with a measure μ, acting in a complex Hilbert space $\mathfrak{K}$. Then there exists a unique complex Hilbert space $\mathfrak{K}_K$ of equivalence classes with respect to μ of mappings of X into $\mathfrak{K}$ satisfying the following conditions:

(1) The set $\mathfrak{G}_K = \{[K(\cdot,y)\phi] \mid y \in X \text{ and } \phi \in \mathfrak{K}\}$ is total in $\mathfrak{K}_K$.

(2) There exists a μ-selection σ such that the linear mapping

$$E_x^K : [f] \mapsto \sigma([f])(x)$$

of $\mathfrak{K}_K$ into $\mathfrak{K}$ is continuous for all $x \in X$ and $E_x^K E_y^{K*} = K(x,y)$ for all x,y in X.

If $K(\cdot,y)$ is μ-measurable in X for all $y \in X$ then $\mathfrak{K}_K$ is a Hilbert space of equivalence classes of μ-measurable mappings; K is an admissible square-integrable positive μ-kernel if and only if $\mathfrak{K}_K$ is a Hilbert subspace of $L^2_{\mathfrak{K}}(X,\mu)$. Moreover, if $K(\cdot,y)$ is continuous in X for all $y \in X$ when $\mathscr{L}(\mathfrak{K})$ is equipped with the strong operator topology, then $\mathfrak{K}_K$ can be identified with the unique complex Hilbert space of continuous mappings of X into $\mathfrak{K}$ which satisfies (1) and (2) with obvious modifications (cf. Ref. 14, Theorem 1).

Proof: Let $\mathrm{sp}(\mathfrak{G}_K)$ be the linear span of $\mathfrak{G}_K$ in $F(X;\mathfrak{K})$. By virtue of (III.1) (cf. Remark 4), there exists a (unique) positive Hermitian sesquilinear form $(\cdot|\cdot)$ on $\mathrm{sp}(\mathfrak{G}_K)$ such that

$$([K(\cdot,y)\phi] \mid [K(\cdot,z)\psi]) = (K(z,y)\phi \mid \psi)_{\mathfrak{K}} \tag{III.3}$$

for all y,z in X and all ϕ,ψ in $\mathfrak{K}$. Note that (III.3) is meaningful because K is admissible: in fact, if $[K(\cdot,y')\phi'] = [K(\cdot,y)\phi]$ and $[K(\cdot,z')\psi'] = [K(\cdot,z)\psi]$, we have

$$(K(z',y')\phi'|\psi')_{\mathfrak{K}} = (K(z',y)\phi|\psi')_{\mathfrak{K}} = (\phi|K(y,z')\psi')_{\mathfrak{K}}$$
$$= (\phi|K(y,z)\psi)_{\mathfrak{K}} = (K(z,y)\phi|\psi)_{\mathfrak{K}}.$$

It follows then from the Cauchy–Schwarz inequality that $(\cdot|\cdot)$ is nondegenerate. For let $f = \sum_j K(\cdot,x_j)\phi_j$ $(x_j \in X;\ \phi_j \in \mathfrak{K})$ with a finite sum; for each $x \in X$ we have, using (III.3),

$$\begin{aligned}\|f(x)\|^2_{\mathfrak{K}} &= \sum_{j,k}(K(x,x_j)\phi_j|K(x,x_k)\phi_k)_{\mathfrak{K}}\\ &= \sum_{j,k}([K(\cdot,x_j)\phi_j]|[K(\cdot,x)K(x,x_k)\phi_k])\\ &\leqslant \|[f]\|\ \left\|\left[\sum_j K(\cdot,x)K(x,x_j)\phi_j\right]\right\|\\ &\leqslant \|[f]\|(K(x,x)f(x)|f(x))_{\mathfrak{K}}^{1/2},\end{aligned}$$

whence

$$\|f(x)\|_{\mathfrak{K}} \leqslant \|[f]\|\ \|K(x,x)\|^{1/2} \tag{III.4}$$

and $f(x) = 0$ whenever $\|[f]\| = 0$. In addition, (III.4) implies that for every Cauchy sequence $([f_n])$ in $\mathrm{sp}(\mathfrak{G}_K)$ with

$$f_n = \sum_{j \in J_n} K(\cdot,x_j)\phi_j,$$

where J_n is some finite index set, the sequence (f_n) converges pointwise in $\mathscr{F}(X;\mathfrak{K})$. Thus $\mathrm{sp}(\mathfrak{G}_K)$ is dense in a unique complete vector subspace of $F(X;\mathfrak{K})$. Equipped with the scalar multiplication $(\cdot|\cdot)_K$ which extends $(\cdot|\cdot)$, this subspace is the wanted Hilbert space $\mathfrak{K}_K$.

To show that condition (2) is satisfied, we choose a μ-selection σ continuous in $\mathfrak{K}_K$ when $\mathscr{F}(X;\mathfrak{K})$ is endowed with the topology of pointwise convergence and such that

$$\sigma([K(\cdot,y)\phi]) = K(\cdot,y)\phi$$

for all $y \in X$ and all $\phi \in \mathfrak{K}$. This choice makes sense because K is admissible. Moreover, for each $x \in X$, the mapping $[f] \mapsto \sigma([f])(x)$ of $\mathrm{sp}(\mathfrak{G}_K)$ into $\mathfrak{K}$ is continuous by (III.4) and can be uniquely extended to a continuous linear mapping of $\mathfrak{K}_K$ into $\mathfrak{K}$. It follows that the mapping E^K_x is continuous and that

$$(K(x,y)\phi|\psi)_{\mathfrak{K}} = (E^K_x[K(\cdot,y)\phi]|\psi)_{\mathfrak{K}} = ([K(\cdot,y)\phi]|E^{K*}_x\psi)_K$$

for all x,y in X and all ϕ,ψ in $\mathfrak{K}$, where E^{K*}_x is the (continuous) adjoint of E^K_x. Using (III.3), we get

$$E^{K*}_x\psi = [K(\cdot,x)\psi], \tag{III.5}$$

whence $E^K_x E^{K*}_y = K(x,y)$.

The assertion about the μ-measurability follows from Egoroff's theorem (Ref. 5, Chap. 4, § 5, Theorem 2) and from (Ref. 5, Chap. 4, § 5, Proposition 6). If K is an admissible square-integrable positive μ-kernel, then, by virtue of (III.2), $\mathrm{sp}(\mathfrak{G}_K)$ equipped with the scalar multiplication $(\cdot|\cdot)$ is a pre-Hilbert subspace of $L^2_{\mathfrak{K}}(X,\mu)$ whose closure is $\mathfrak{K}_K$. The converse is straightforward. In the case where $K(\cdot,y)$ is continuous for all $y \in X$, every element of $\mathfrak{K}_K$ contains a continuous mapping defined by means of K (Ref. 14, Theorem 1); the space of all these mappings identifies to $\mathfrak{K}_K$ in an obvious way.■

Remark 5: It follows from (III.5) that E^{K*}_x, and therefore E^K_x, is uniquely defined by K for all $x \in X$. This justifies, *a posteriori*, the superscript "K."

Corollary: Let X,μ,K, and $\mathfrak{K}$ be as in Proposition 3. Then

(i) K is reproducing in $\mathfrak{K}_K$, i.e., for each $y \in X$, each $\phi \in \mathfrak{K}$, and each $[f] \in \mathfrak{K}_K$, we have

$$([K(\cdot,y)\phi]|[f])_K = (\phi|E^K_y[f])_{\mathfrak{K}}.$$

(ii) For each $(x,y) \in X \times X$ we have

$$\|K(x,y)\|^2 \leqslant \|K(x,x)\|\,\|K(y,y)\|.$$

Proof: Assertion (i) follows from (III.5). From (III.4), with $f = K(\cdot,y)\phi$ $(y \in X;\ \phi \in \mathfrak{K})$, we obtain

$$\|K(x,y)\phi\|^2_{\mathfrak{K}} \leqslant \|[K(\cdot,y)\phi]\|^2_K\|K(x,x)\|,$$

i.e.,

$$(K(x,y)^*K(x,y)\phi|\phi)_{\mathfrak{K}} \leqslant (K(y,y)\phi|\phi)_{\mathfrak{K}}\|K(x,x)\|,$$

whence assertion (ii). ■

Proposition 4: Let X,μ, and $\mathfrak{K}$ be as in Proposition 3. If $\mathfrak{H}$ is a complex Hilbert space of equivalence classes with respect to μ of mappings of X into $\mathfrak{K}$, then the following conditions are equivalent:

(i) There exists an admissible positive μ-kernel K on X acting in $\mathfrak{K}$ such that $\mathfrak{K}_K = \mathfrak{H}$.

(ii) There exists a μ-selection σ such that, for each $x \in X$, the linear mapping

$$E_x : [f] \mapsto \sigma([f])(x)$$

of $\mathfrak{H}$ into $\mathfrak{K}$ is continuous.

Proof: (i) $\Rightarrow$ (ii): This follows from Proposition 3 with $E_x = E^K_x$.

(ii) $\Rightarrow$ (i): Since E_x is continuous for all $x \in X$, its adjoint E^*_x is continuous; hence we have a mapping K of $X \times X$ into $\mathscr{L}(\mathfrak{K})$ defined by

$$K(x,y) = E_x E^*_y. \tag{III.6}$$

This mapping is a positive μ-kernel on X acting in $\mathfrak{K}$, for, if J is any finite index set, then

$$\sum_{j\in J,k\in J}(K(x_k,x_j)\phi_j|\phi_k)_{\mathfrak{K}} = \sum_{j\in J,k\in J}(E_{x_k}E^*_{x_j}\phi_j|\phi_k)_{\mathfrak{K}} = \Big\|\sum_{j\in J}E^*_{x_j}\phi_j\Big\|^2_{\mathfrak{K}} \geqslant 0$$

for all x_j,x_k in X and all ϕ_j,ϕ_k in $\mathfrak{K}$. Now, for each pair x,y of elements of X and for each $\phi \in \mathfrak{K}$, we have

$$K(x,y)\phi = E_x E^*_y\phi = \sigma(E^*_y\phi)(x);$$

thus $E^*_y\phi = [K(\cdot,y)\phi]$ and K is admissible. On the other hand, if $(E^*_y\phi|[f])_{\mathfrak{H}} = 0$ for all $y \in X$, all $\phi \in \mathfrak{K}$, and a certain $[f] \in \mathfrak{H}$, then $(\phi|\sigma([f])(y))_{\mathfrak{K}} = (E^*_y\phi|[f])_{\mathfrak{H}} = 0$, whence $\sigma([f]) = 0$ and $[f] = 0$. Therefore, condition (1) of Proposition 3 is satisfied and, as condition (2) is fulfilled by assumption and by (III.6), with $E^K_x = E_x$ $(x \in X)$, assertion (i) follows from Proposition 3.■

Corollary: If X is a locally compact space equipped with a nontrivial measure μ and if $\mathfrak{K}$ is a complex Hilbert space, then the mapping $I:(x,y) \mapsto \mathrm{Id}_{\mathfrak{K}}$ of $X \times X$ into $\mathscr{L}(\mathfrak{K})$ is an admissible positive μ-kernel on X acting in $\mathfrak{K}$ such that $\mathfrak{K}_I$ is isomorphic to $\mathfrak{K}$. When, in addition, X is compact and μ positive, the admissible positive μ-kernel $(1/\mu(X))I$ is square-integrable.

Proof: The complex vector space $\mathfrak{L}$ of the equivalence classes with respect to μ of all constant mappings of X into $\mathfrak{K}$

becomes a Hilbert space isomorphic to $\mathfrak{K}$ when equipped with the scalar multiplication $(\cdot|\cdot)_{\mathfrak{L}}$ defined by

$$([f]\,|\,[f'])_{\mathfrak{L}} = (f(x)|f'(x))_{\mathfrak{K}},$$

where f,f' are arbitrary constant mappings of X into $\mathfrak{K}$ and x is any element of X. The μ-selection σ defined by $\sigma([f]) = f$, where f is any constant mapping of X into $\mathfrak{K}$, makes the evaluation mapping $E_x: [f] \mapsto \sigma([f])(x)$ continuous for all $x \in X$ and we have $E_x E_y^* = \mathrm{Id}_{\mathfrak{K}}$ for all x,y in X; hence $\mathfrak{K}_I = \mathfrak{L}$. ■

Remark 6: In what precedes, we never have excluded the possibility of getting $[K(\cdot,y)\phi] = [K(\cdot,y)\psi]$ with $\phi \neq \psi$ for a given $y \in X$, i.e., $E_y^{K*}\phi = E_y^{K*}\psi$. It is easy to check that, for an arbitrary $y \in X$, the following conditions are equivalent:

(i) E_y^{K*} is injective.

(ii) E_y^K has a dense range in $\mathfrak{K}$.

(iii) $K(y,y)$ is strictly positive.

Remark 7: Let K be an admissible square-integrable positive μ-kernel on X acting in $\mathfrak{K}$; then we have

$$([f]\,|\,[f'])_K = \int (E_x^K[f]\,|\,E_x^K[f'])_{\mathfrak{K}}\, d\mu(x)$$

for all $[f]$, $[f']$ in $\mathfrak{K}_K$. If μ is positive, the mapping $M: \mathscr{B}_X \mapsto \mathscr{L}(\mathfrak{K}_K)$ given by

$$M(B) = \int \phi_B(x) M_x\, d\mu(x) \quad \textit{weakly},$$

where $M_x = E_x^{K*}E_x^K$, is an observable in $\mathfrak{K}_K$ based on X which admits a μ-density $D_M: x \to M_x$ defined everywhere in X. If for any continuous operator A in $\mathfrak{K}_K$, we define a mapping A^K of $X \times X$ into $\mathscr{L}(\mathfrak{K})$ by

$$A^K(y,x) = E_y^K A E_x^{K*},$$

we obtain

$$E_y^K A\,[f] = \int A^K(y,x) E_x^K[f]\, d\mu(x) \quad \textit{weakly}$$

for all $[f] \in \mathfrak{K}_K$ and all $y \in X$. In fact, for each $\phi \in \mathfrak{K}$, we have

$$\begin{aligned}(E_y^K A\,[f]\,|\,\phi)_{\mathfrak{K}} &= ([f]\,|\,A^* E_y^{K*}\phi)_K \\ &= \int (E_x^K[f]\,|\,E_x^K A^* E_y^{K*}\phi)_{\mathfrak{K}}\, d\mu(x) \\ &= \int (A^K(y,x) E_x^K[f]\,|\,\phi)_{\mathfrak{K}}\, d\mu(x).\end{aligned}$$

IV. DENSITIES

Equipped with the results of Sec. III, we now can establish a connection between the existence of a density of a covariant observable acting in $\mathfrak{H}$ and the existence of a kernel Hilbert space isomorphic to $\mathfrak{H}$.

Proposition 5: Let G be a locally compact group, let H be a closed subgroup of G, and let μ be a nontrivial positive G-quasi-invariant measure on G/H defined by a ρ-function. Given a complex Hilbert space $\mathfrak{H}$ carrying a strongly continuous unitary representation U of G and an observable M in $\mathfrak{H}$ based on G/H which is G-covariant with respect to U, let $V: \mathfrak{H} \to L^2_{\mathfrak{K}}(G/H,\mu;\gamma(U))$ be the isometric mapping of Proposition 2. Then the following conditions are equivalent:

(i) M admits a μ-density $D_M: x \mapsto M_x$.

(ii) There exists an admissible positive μ-kernel K on G/H acting in $\mathfrak{K}$ such that $\mathfrak{K}_K = V\mathfrak{H}$.

Proof: (i) $\Rightarrow$ (ii): Since

$$M(B) = \int \phi_B(x) M_x\, d\mu(x) \quad \textit{weakly} \quad (B \in \mathscr{B}_{G/H}),$$

then, for each $[f] \in V\mathfrak{H}$ and each $B \in \mathscr{B}_{G/H}$, we have

$$\begin{aligned}(M(B)V^*[f]\,|\,V^*[f])_{\mathfrak{H}} &= (P_{\mathfrak{K}}(B)[f]\,|\,[f])_{L^2} \\ &= \int \phi_B(x) \|E_x[f]\|^2_{\mathfrak{K}}\, d\mu(x) \\ &= \int \phi_B(x) \|M_x^{1/2} V^*[f]\|^2_{\mathfrak{H}}\, d\mu(x),\end{aligned}$$

where E_x is the evaluation mapping at x defined by an arbitrary μ-selection. It follows that

$$\|E_x[f]\|_{\mathfrak{K}} = \|M_x^{1/2} V^*[f]\|_{\mathfrak{H}} \leq \|M_x^{1/2}\|\ \|[f]\|_{V\mathfrak{H}} \quad \mu(x)\text{-a.e.} \tag{IV.1}$$

Since (II.5) can be translated as

$$E_x(\mathrm{Ind}_H^G \gamma(U))(g) = \alpha(g^{-1},x)^{1/2} E_{g^{-1}\cdot x} \tag{IV.2}$$

for all $x \in G/H$ and all $g \in G$, we see that E_x is continuous in $V\mathfrak{H}$ for all $x \in G/H$. By Proposition 4, there exists an admissible positive μ-kernel K on G/H acting in $\mathfrak{K}$ such that $\mathfrak{K}_K = V\mathfrak{H}$ and $E_x = E_x^K$ for all $x \in X$. In addition, it follows from (IV.1) that

$$M_x = V^* E_x^* E_x V \quad (x \in X).$$

(ii) $\Rightarrow$ (i): By Proposition 4, the linear mapping E_x^K is continuous for all $x \in G/H$. Since

$$\begin{aligned}&\int \phi_B(x) (V^* E_x^{K*} E_x^K V\phi\,|\,\phi)_{\mathfrak{H}}\, d\mu(x) \\ &= \int \|\phi_B(x) E_x^K V\phi\|^2_{\mathfrak{K}}\, d\mu(x) \\ &= \|P_{\mathfrak{K}}(B) V\phi\|^2_{L^2} = (M(B)\phi\,|\,\phi)_{\mathfrak{H}}\end{aligned}$$

for all $B \in \mathscr{B}_{G/H}$ and all $\phi \in \mathfrak{H}$, the observable M admits a μ-density

$$D_M: x \mapsto M_x = V^* E_x^{K*} E_x^K V$$

defined everywhere in G/H. ■

Remark 8: It follows from the proof of Proposition 5 that E_x^K is continuous for all $x \in G/H$ so that we can choose a μ-density $D_M: x \mapsto M_x$ defined everywhere in G/H and satisfying

$$M_{g\cdot x} = \alpha(g,x)^{-1} U(g) M_x U(g)^{-1} \tag{IV.3}$$

for all $g \in G$ and all $x \in G/H$. In addition, by (IV.2) we have

$$\begin{aligned}K(g\cdot x, g\cdot y) = E_{g\cdot x}^K E_{g\cdot y}^{K*} &= \alpha(g,x)^{-1/2}\alpha(g,y)^{-1/2} E_x^K E_y^{K*} \\ &= \alpha(g,x)^{-1/2}\alpha(g,y)^{-1/2} K(x,y)\end{aligned} \tag{IV.4}$$

for all $g \in G$ and all x,y in G/H, and we can say that *K is G-quasi-invariant*.

If μ is G-invariant, then (IV.3) becomes

$$M_{g\cdot x} = U(g) M_x U(g)^{-1} \tag{IV.5}$$

and (IV.4)

$$K(g\cdot x, g\cdot y) = K(x,y),$$

i.e., *K is G-invariant*. It follows now from (IV.5) that if there exists $x_1 \in G/H$ such that M_{x_1} is a projection, then M_x is a projection with the same rank of M_{x_1} for all $x \in G/H$ (cf. Remark 3).

By choosing $x = x_0 = H$ in (IV.3) and (IV.5), we see that D_M is completely determined by $M_{x_0} \in \mathscr{L}(\mathfrak{H})^+$, the representation U, and the function α. For each $h \in H$ we have, by virtue of (II.3),

$$U(h)M_{x_0} = (\Delta_H(h)/\Delta_G(h))M_{x_0}U(h)$$

and, if μ is G-invariant,

$$U(h)M_{x_0} = M_{x_0}U(h).$$

The following Corollary 1 extends to every locally compact group G a result already known for G compact and second countable (Ref. 2, 4.5, Theorem 5.3).

Corollary 1: Let $G,H,\mu,\mathfrak{H},U$, and M be as in Proposition 5. If $\mathfrak{H}$ is finite-dimensional, then M admits a μ-density.

Proof: The linear mapping E_x of Proposition 5 is continuous for all $x \in G/H$ because $V\mathfrak{H}$ is finite-dimensional. ■

Corollary 2: Let $G,H,\mu,\mathfrak{H},U$, and M be as in Proposition 5. If G is second countable, μ is diffuse, $\mathfrak{H}$ is infinite-dimensional, and M is a decision observable, then M does not admit a μ-density.

Proof: We use the notation of Proposition 5 and assume that M admits a μ-density defined everywhere in G/H. Let C be a compact subset of G/H with $\mu(C) > 0$; put

$$\alpha = \sup_{x \in C} \|E_x^K\|,$$

and define, for each $\phi \in \mathfrak{K}$, a mapping $f^\#$ of G into $\mathfrak{K}$ by

$$f^\#(s(x)h) = U_0(h)^{-1}\phi_{C_0}(x)\phi \quad (x \in G/H; h \in H),$$

where s is any Borel section associated with the canonical mapping of G onto G/H, $U_0 = \gamma(U)$, and C_0 is a μ-integrable subset of C such that $0 < \mu(C_0) < 1/\alpha^2$ (which exists because μ is diffuse). Then, with $f = f^\# \circ s$, we have $[f] \in L^2_{\mathfrak{K}}(G/H,\mu;U_0)$; moreover, $\|E_x^K[f]\|_{\mathfrak{K}} = \|\phi\|_{\mathfrak{K}}$ $\mu(x)$-a.e. in C_0. If we choose ϕ such that $\|\phi\|^2_{\mathfrak{K}} = 1/\mu(C_0)$, then we have $\|[f]\|_{L^2} = 1$ and $\|E_x^K[f]\|_{\mathfrak{K}} > \alpha$ $\mu(x)$-a.e. in C_0, which is impossible. ■

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Regge trajectories in confining potentials

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The analyticity of the energy level $E_n(l)$ in the half-plane $\mathrm{Re}(l) > -\frac{1}{2}$ has been proved for some interesting superpositions of quark-confining potentials.

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I. INTRODUCTION

Recently Grosse and Martin[1] (GM) initiated the study of Regge trajectories in confining potentials. They proved that for pure power-law potentials

$$V(r) = r^\alpha, \ \alpha > 0 \tag{1}$$

the energy levels $E_n(l)$ in the complex angular momentum (l) plane are analytic for $\mathrm{Re}(l) > -\frac{1}{2}$. It would be interesting to extend the above theorem for a class of potentials of the form

$$V(r) = \int_{-2}^{\infty} \rho(\alpha) r^\alpha \, d\alpha, \quad \rho \geqslant 0 \text{ when } \alpha > 0. \tag{2}$$

But as remarked by GM, their technique is unsuitable for superposition of potentials. However, a slight extension of the GM technique could prove the desired analyticity of $E_n(l)$ in the half-plane $\mathrm{Re}(l) > -\frac{1}{2}$ for the class of potentials

$$V(r) = r + kr^\beta, \ k > 0, 0.4 < \beta < 1. \tag{3}$$

This is done in Sec. II. As will be clear the proof actually holds for

$$V(r) = r^\alpha + kr^\beta, k > 0, \tag{4}$$

with appropriate bounds on β. In Sec. III we present another method of proving the analyticity of $E_n(l)$ for the class of potentials

$$V(r) = r + k\beta r^\beta, \ -2 < \beta < \tfrac{1}{4}. \tag{5}$$

This includes the interesting case of "Charmonium potential" if $\beta = 1$ and $\alpha > 0$. We still lack, however, a proof for the analyticity of $E_n(l)$ in the gap $\frac{1}{4} \leqslant \beta \leqslant \frac{2}{5}$.

II. SUPERPOSITION OF POTENTIALS: CASE I

In this section we follow the GM approach. So we briefly state the results, stressing only the points where modifications are necessary.

(a) For the potential (3) the Schrödinger wavefunction $u(z)$ for any fixed l,E and $k > 0$ is analytic in z, at least in the z plane cut along the negative real axis. It has the asymptotic behavior

$$u/u_0 \to 1 \quad \text{as } z \to \infty, \ u_0 = z^{-1/4},$$
$$\exp\left[-\tfrac{2}{3} z^{3/2} + E z^{1/2} + O(z^{-1/2})\right] \tag{6}$$

for $|\arg z| < \pi$.

(b) It has been shown by GM that $\mathrm{Im} E_n(\lambda)/\mathrm{Im}\lambda > 0$, if $\lambda = l(l+1)$. Hence $E_n(\lambda)$ has no isolated pole or essential singularity in the λ plane cut along $-\frac{1}{4}$ to $-\infty$. The argument which excludes natural boundaries in the case with pure power potential will remain valid in our case. Thus we need only to consider branch points. To discard branch points the strategy is to characterize the energy level for any l by the number of zeros of the corresponding wavefunction in a sector (independent of l) of the z plane.

(i) Let λ be real and $\lambda > -\frac{1}{4}$. The Schrödinger equation along a ray $z = te^{i\phi}$ is $(2\mu = \hbar = 1)$

$$\left(-\frac{d^2}{dt^2} + \frac{\lambda}{t^2} + te^{3i\phi} + kt^\beta e^{i(2+\beta)\phi}\right)u = Ee^{2i\phi}u, \ k > 0, \ \beta < 1. \tag{7}$$

By multiplying by u^* and integrating, we get

$$\mathrm{Re}(u'u^*) = \int_0^t dt' \left\{ |u'|^2 + |u|^2 \left[\frac{\lambda}{t'^2} + t'\cos 3\phi + kt'^\beta \cos(2+\beta)\phi - E\cos 2\phi \right] \right\}, \tag{8}$$

$$\mathrm{Im}(u'u^*) = \int_0^t dt' |u|^2 [t'\sin 3\phi + kt'^\beta \sin(2+\beta)\phi - E\sin 2\phi]. \tag{9}$$

If $|\phi| < \pi/3$, $u \to 0$ as $t \to \infty$ and the integration sign $\int_0^t$ in (9) can be replaced by $-\int_t^\infty$. In this case the integrand in (9) is monotonically increasing (decreasing) if $\phi > 0$ $(\phi < 0)$. So we can choose the limits in such a way that the integrand assumes a constant sign. Hence $\mathrm{Im}(u'u^*) \neq 0$ which shows that u has not zero in $0 < |\phi| < \pi/3$. Next we consider the combination

$$\mathrm{Re}(u'u^*)\cos\gamma - \mathrm{Im}(u'u^*)\sin\gamma. \tag{10}$$

It will be different from zero if we can find γ such that

$$\cos\gamma > 0, \ \cos(3\phi + \gamma) > 0,$$
$$\cos[(2+\beta)\phi + \gamma] > 0, \ \cos(2\phi + \gamma) < 0. \tag{11}$$

The inequalities hold uniformly provided we choose

$$\pi/3 \leqslant |\phi| < \pi \quad \text{and} \quad 0 < \beta < 1.$$

Hence we get

Lemma 2.1: For a real $\lambda > -\frac{1}{4}$ and $0 < \beta < 1$, u has no zero in $0 < |\phi| < \pi$.

(ii) Let λ be complex. Choose, for instance, $\mathrm{Im}\,\lambda > 0$. Equation (9) becomes

$$\mathrm{Im}(u'u^*) = \int_0^t dt' |u|^2 \left[\frac{\mathrm{Im}\lambda}{t'^2} + t'\sin 3\phi + kt'^\beta \sin(2+\beta)\phi - |E|\sin(2\phi + \arg E) \right]. \tag{12}$$

If $0 < \phi < \pi/3$, the integral tends to zero if $t \to \infty$. Moreover, $\sin 3\phi > 0$, $\sin(2+\beta)\phi > 0$. So we have $\sin(2\phi + \arg E) > 0$. Hence we conclude that

$$0 < \arg E < \pi/3, \ \mathrm{Im}\lambda > 0. \tag{13}$$

Also an argument similar to that applied in the proof of Lemma 2.1 shows that

Lemma 2.2: For $\mathrm{Im}\lambda > 0$, u has no zero for $-\pi/3 < \phi \leqslant 0$.□ We now prove the following

Lemma 2.3: For $\mathrm{Im}\lambda > 0$, u has no zero for $\phi = 5\pi/6$ if we restrict β in $0.4 < \beta < 1$. Also u has no zero for t large enough and $|\phi| < \pi$.

Proof: Here we can only use the limit $(0,t)$:

$$\mathrm{Im}(u'u^*) = \int_0^t dt'|u|^2\Big[\frac{\mathrm{Im}\lambda}{t'^2} + t' + kt'^\beta \sin(2+\beta)\frac{5\pi}{6} - |E|\sin\Big(\frac{5\pi}{3} + \arg E\Big)\Big]. \tag{14}$$

According to (13), we have $\pi < 5\pi/3 + \arg E < 2\pi$. Hence the integrand is positive if we have $\sin(2+\beta)5\pi/6 > 0$. This gives the bounds on β: $\frac{2}{5} < \beta < 1$. The upper bound is chosen to meet the boundary condition at infinity. This proves the first part of the lemma. The second part follows from the Eq. (6).

We have thus proved that, for real $\lambda > -\frac{1}{4}$, $u(z)$ has only n real zeros (corresponding to the nth level E_n) and no other zero in the sector $|\phi| < \pi$. For complex λ (with, for instance, $\mathrm{Im}\lambda > 0$) there are no zeros in $-\pi/3 < \phi \leqslant 0$, no zeros on the line $\phi = 5\pi/6$, and no zeros at infinity in the sector $0 < |\phi| < \pi$. Hence, if we vary λ continuously starting from and returning to a point on the λ real axis the number of zeros cannot change and we get back the same energy level. Thus $E_n(\lambda)$ has no branch point in the cut λ plane. Hence we conclude

Theorem 2.1: The energy level $E_n(l)$ in the potential $V(r) = r + kr^\beta$, $k > 0$, $0.4 < \beta < 1$ is analytic in $\mathrm{Re}(l) > -\frac{1}{2}$.

The proof can also be extended to potentials $V(r) = r^\alpha + kr^\beta$, $k > 0$, $2\alpha/(4+\alpha) < \beta < \alpha < 4$.

III. SUPERPOSITION OF POTENTIALS: CASE II

We now consider the class of potentials

$$V(r) = r + k\beta r^\beta, \tag{5}$$

where k is any real number. The special choice of the coupling parameter does not reduce the generality of the class of potentials. To prove the anlyticity of the energy eigenvalue $E_n(l)$ *in* $\mathrm{Re}(l) > -\frac{1}{2}$ we need, in this section, the following result.

Theorem 3.1: The energy eigenvalue (E_n) in the potential (5) is analytic in β for $-2 < \beta < \frac{1}{4}$ for any fixed l in the half-plane $\mathrm{Re}(l) > -\frac{1}{2}$. Moreover, for β in this interval, the energy eigenvalues are nondegenerate.

We shall prove this theorem using the well-known Kato–Rellich theory. Let us denote

$$\tau = \frac{d^2}{dr^2} + \frac{\lambda}{r^2} + r + k\beta r^\beta, \ \lambda = l(l+1), \tag{15}$$

which is a formal differential operator. At the beginning we restrict β only by the inequality $\beta > -2$. Then with real $l > -\frac{1}{2}$, τ defined as an operator in $L^2(0,\infty)$ is of the limit-point type at infinity for all values of l, limit-circle type for $-\frac{1}{2} < l < \frac{1}{2}$ and limit-point type for $l \geqslant \frac{1}{2}$ at the origin. Hence for the self-adjoint extension of the symmetric operator τ in $L^2(o,\infty)$ we need a boundary condition at $r = 0$ which corresponds to the usual normalization condition $\lim_{r\to 0} r^{-l-1}u = 1$, u belonging to the domain of τ. We thus have

Definition 3.1: The operator family $H(\beta,\lambda)$ is the unique self-adjoint extension of the symmetric operator τ in $L^2(0,\infty)$, and it is defined on the dense domain $D(H)$ which is the set of all $u \in L^2(0,\infty)$ such that $du/dr \in L^2(0,\infty)$, $u(0) = 0$, and $\tau u \in L^2(0,\infty)$. For complex l with $\mathrm{Re}(l) > -\frac{1}{2}$, $H(\beta,\lambda)$ will be defined on $D(H)$ as a closed operator with the following property

$$H(\beta,\lambda)^* = H(\beta,\bar{\lambda}],$$

where $H(\beta,\lambda)^*$ is the adjoint of $H(\beta,\lambda)$.

Let us denote by $\tilde{V}$ the maximal multiplication operator r^β in $L^2(0,\infty)$.

Lemma 3.1: $\tilde{V}$ *is* $H(0,\lambda)$-compact for $-2 < \beta < \frac{1}{4}$ uniformly in l lying in any compact set in $\mathrm{Re}(l) > -\frac{1}{2}$.

Proof: Our proof follows a similar approach of Graffi *et al.*[2] We first note that the kernel of the integral operator $H(0,\lambda)^{-1}$ is given by the Green's function

$$G(x,y) = \begin{cases} f_\nu(x)g_\nu(y), & x \leqslant y, \\ f_\nu(y)g_\nu(x), & y \leqslant x, \end{cases}$$

where

$$f_\nu(x) = (\tfrac{2}{3}x)^{1/2} I_\nu(\tfrac{2}{3}x^{3/2}),$$
$$g_\nu(x) = (\tfrac{2}{3}x)^{1/2} K_\nu(\tfrac{2}{3}x^{3/2}), \quad \nu = \tfrac{1}{3}(2l+1).$$

I_ν and K_ν are modified Bessel functions. Hence the kernel of the operator $\tilde{V}H(0,\lambda)^{-1}$ is given by $x^\beta G(x,y)$. Now it can be shown (see Appendix) that

$$\int_0^\infty \int_0^\infty |x^\beta G(x,y)|^2 dx dy < \infty$$

uniformly in β and l on compact sets in the interval $-2 < \beta < \frac{1}{4}$ and in the half-plane $\mathrm{Re}(l) > -\frac{1}{2}$, respectively. Thus $\tilde{V}H(0,\lambda)^{-1}$ is a Hilbert–Schmidt operator and hence compact. We note incidentally that $H(0,\lambda)^{-1}$ itself is a compact operator which follows for $\beta = 0$ in $\tilde{V}$. The above observations prove the lemma.[3]

Corollary to Lemma 3.1: For any fixed l in $\mathrm{Re}(l) > -1/2$, $H(\beta,\lambda)$ is a holomorphic family of type A in β for $-2 < \beta < \frac{1}{4}$ and it has compact resolvent.

Proof: $\tilde{V}$ is $H(0,\lambda)$-compact implies that $\tilde{V}$ is $H(0,\lambda)$-bounded with relative bound zero for $-2 < \beta < \frac{1}{4}$. Hence by standard arguments,[4] the result follows.

As a consequence of the corollary every nondegenerate eigenvalue of $H(\beta,\lambda)$ is analytic in β near $\beta = \beta_0$ with $\beta_0 \in (-2, \frac{1}{4})$.

Lemma 3.2: Consider an operator

$$P(\beta) = -(2\pi i)^{-1}\int_C [H(\beta,\lambda) - z]^{-1} dz,$$

where C encloses only $E_n = E_n(0)$ and no other eigenvalue of $H(0,\lambda)$. Then $P(\beta)$ is bounded holomorphic in β in $-2 < \beta < \frac{1}{4}$ for each l in $\mathrm{Re}(l) > -\frac{1}{2}$ and so $P(\beta)$ is the projection operator corresponding to $E_n(\beta)$. Also for each β in $-2 < \beta < \frac{1}{4}$ the dimension of the range space of $P(\beta)$ is 1.

Proof: The proof will be given in two steps.

Step 1: The operator

$$P = (2\pi i)^{-1}\int_C [H(0,\lambda) - z]^{-1} dz$$

is the projection operator corresponding to E_n for each fixed l in $\text{Re}(l) > -\frac{1}{2}$. Since E_n is analytic[1] in $\text{Re}(l) > -\frac{1}{2}$, $H(0,\lambda)$ is nondegenerate in $\text{Re}(l) > -1/2$ and so

$$\dim[\text{range } P] = 1. \tag{16}$$

Now,

$$[H(\beta,\lambda) - z]^{-1}$$
$$= [H(0,\lambda) - z]^{-1}\{1 + k\beta r^\beta [H(0,\lambda) - z]^{-1}\}^{-1}. \tag{17}$$

Hence the lhs of (17) is holomorphic provided

$$\|k\beta r^\beta [H(0,\lambda) - z]^{-1}\| < 1.$$

We write,

$$\|r^\beta H(0,\lambda)^{-1}\| = N(\beta),\ \ \|[1 - zH(0,\lambda)^{-1}]^{-1}\| = M(z),$$

$$N_0 = \inf_{-2<\beta<1/4} N(\beta),\ \ M_0 = \inf_{z\in C} M(z).$$

Then with the choice

$$|k| < 1/2M_0N_0 \tag{18}$$

we see that $[H(\beta,\lambda) - z]^{-1}$ and hence $P(\beta)$ is holomorphic in $-2<\beta<\frac{1}{4}$ for each l in $\text{Re}(l) > -\frac{1}{2}$. Also the dimension of the range of $P(\beta)$ is 1, which follows, by continuity, from (16). Hence the lemma is proved for small k satisfying (18).

Step 2: The lemma, however, holds for any k. To show that we first note that Step 1 is true actually for potentials

$$V(r) = \rho r + k\beta r^\beta,\ \rho > 0. \tag{19}$$

[In fact, all our earlier resutls remain true for (19). We chose $\rho = 1$ only for the convenience of notation.] Here the bound corresponding to (18) is independent of ρ, since in the present case the infimum of $N(\beta,\rho)$ and $M(z,\rho)$ are taken also on ρ on a compact set. Now the well-known Symanzik scaling law gives

$$E_n(1,\eta) = \rho^{-2/3}E_n(\rho,k),$$
$$\eta = k\rho^{-(\beta+2)/3}. \tag{20}$$

We suppress the β dependence in E_n for convenience. Choose ρ small and $|k| < \frac{1}{2}M_0N_0$. Then the projection $P_\rho(\beta)$ corresponding to $E_n(\rho,k)$ is holomorphic in β and $\dim[\text{range } P_\rho(\beta)] = 1$. Hence Eq. (20) shows that $P(\beta)$ corresponding to $E_n(1,\eta)$ is also holomorphic in β and $\dim[\text{range } P(\beta)] = 1$ for

$$|\eta| < \frac{1}{2M_0N_0}\rho^{-(\beta+2)/3}. \tag{21}$$

Since ρ is small and arbitrary, (21) implies that $|\eta|$ would be arbitrary but a finite number. In otherwords $P(\beta)$ corresponding to $E_n(1,\eta)$ is holomorphic in β for any finite real η. This proves the lemma.

Lemma 3.2 means that $H(\beta,\lambda)$, l fixed with $\text{Re}(l) > -\frac{1}{2}$, is nondegenerate for $-2<\beta<\frac{1}{4}$. So each eigenvalue $E_n(\beta)$ is nondegenerate. This together with the remark below the corollary to Lemma 3.1 completes the proof of Theorem 3.1.

We are now in a position to prove the main result. As remarked in Sec. II, it is only necessary to show the nonexistence of branch points and natural boundaries in the energy eigenvalue as a function of l in $\text{Re}(l) > -\frac{1}{2}$. Let us first exclude branch points. We do this by constructing a contradiction. We begin by writing two Schrödinger equations

$$-u_n'' + \left(\frac{\lambda}{r^2}\right)u_n = E_n u_n, \tag{22}$$

$$-v_n'' + \left(\frac{\lambda}{r^2} + r + k\beta r^\beta\right)v_n = \epsilon_n v_n,\ \ -2<\beta<\tfrac{1}{4}, \tag{23}$$

where $\lambda = l(l+1)$. According to Theorem 3.1, $E_n(\beta,\lambda)$ is analytic in β for $-2<\beta<\frac{1}{4}$ for any fixed λ in the λ plane cut along $-\frac{1}{4}$ to $-\infty$ and $\epsilon_n(0,\lambda) = E_n(\lambda)$ for each n. We also know that $E_n(\lambda)$ is analytic in λ in the cut plane. Let us suppose that, for a nonzero β, $\epsilon_n(\beta,\lambda)$ as a function of λ has a branch point at $\lambda = \lambda_0$. Hence, after a complete revolution around $\lambda = \lambda_0$, the Eq. (23) [with λ replaced by λ_0] becomes

$$-v_m'' + \left(\frac{\lambda_0 e^{2i\pi}}{r^2} + r + k\beta r^\beta\right)v_m = \epsilon_m v_m, \tag{24}$$

where $m \neq n$. Now making λ_0 fixed we vary β so that $\beta \to 0$. We thus get [since no two eigenvalues coalesce at $\beta = 0$]

$$-u_m'' + \left(\frac{\lambda_0 e^{2i\pi}}{r^2} + r\right)u_m = \epsilon_m u_m. \tag{25}$$

Equation (22) can also be considered as one obtained from Eq. (23) by letting $\beta \to 0$. Thus, if we assume the existence of a branch point at $\lambda = \lambda_0$ for a nonzero β we arrive at two different Eqs. (22) and (25), respectively, by letting $\beta \to 0$ before and after a complete revolution around $\lambda = \lambda_0$. This means that $\lambda = \lambda_0$ should also be a branch point of $E_n(\lambda)$ which is not the case. Hence the contradiction. Thus $\epsilon_n(\beta,\lambda)$ has no branch point in the cut λ plane if $-2<\beta<\frac{1}{4}$.

Natural boundaries are also automatically discarded. This follows from Theorem 3.1 which states that $\epsilon_n(\beta,\lambda)$ is well-defined for each λ in the cut plane and each β in $-2<\beta<\frac{1}{4}$. Hence we conclude

Theorem 3.2: The energy eigenvalue $\epsilon_n(l)$ in the potential

$$V(r) = r + k\beta r^\beta,\ \ -2<\beta<\tfrac{1}{4}$$

is analytic in l in $\text{Re}(l) > -\frac{1}{2}$.

IV. DISCUSSION

We have proved the analyticity of $E_n(l)$ in the half-plane $\text{Re}(l) > -\frac{1}{2}$ for potentials

$$V(r) = r + k\beta r^\beta$$

in two nonoverlapping regions of β: (i) $\frac{2}{5}<\beta<1$, $k>0$ and (ii) $-2<\beta<\frac{1}{4}$, k real. We are still unable to bridge the gap $\frac{1}{4}\leqslant\beta\leqslant\frac{2}{5}$. However, our proof includes the physically interesting case of the popular Charmonium potential.

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APPENDIX

The proof of the uniform convergence of the integral

$$I = \int_0^\infty\int_0^\infty |x^\beta G(x,y)|^2 dx\, dy \tag{A1}$$

will be given below. The integrand is nonnegative. Also from the asymptotic properties of the Bessel functions I_ν and K_ν the repeated integral

$$\int_0^\infty dx\, x^{2\beta}\int_0^\infty |G(x,y)|^2 dy$$

can be shown to converge uniformly in β in the interval $-2+\eta\leqslant\beta\leqslant\frac{1}{4}-\eta$, $\eta>0$ for each fixed l in $\mathrm{Re}(l)>-\frac{1}{2}$. Hence by Fubinis theorem,[5] the integral I is uniformly convergent in β in the interval $-2+\eta\leqslant\beta\leqslant\frac{1}{4}-\eta$, $\eta>0$ but pointwise convergent in l in $\mathrm{Re}(l)>-\frac{1}{2}$. Explicitly this means that for any $\epsilon>0$ we can find $\delta_1(l)>0$, $\delta_2(l)>0$ and $X_1(l)>0$, $X_2(l)>0$ such that

$$|I-\int_{x'}^{x''}\int_{y'}^{y''}|x_\beta G(x,y)|^2 dxdy|<\epsilon \tag{A2}$$

for $x'<\delta_1(l)$, $y'<\delta_2(l)$, $x''>X_1(l)$, $y''>X_2(l)$ and for all β in $-2+\eta\leqslant\beta\leqslant\frac{1}{4}-\eta$, $\eta>0$.

We next consider the Dixon–Ferrar representation[6] for the Green's function

$$G(x,y)=\tfrac{1}{3}\sqrt{xy}\int_{q_0}^\infty e^{-\nu q}J_0(\tfrac{2}{3}\omega)dq,\quad \mathrm{Re}\nu>0, \tag{A3}$$

where

$$\omega=(-x^3-y^3+2x^{3/2}y^{3/2}\cosh q)^{1/2},$$
$$\cosh q_0=\frac{x^3+y^3}{2x^{3/2}y^{3/2}},\quad \nu=\tfrac{1}{3}(2l+1).$$

Clearly the representation holds uniformly in l in $\mathrm{Re}(l)-\frac{1}{2}$. Inserting the representation in I and using the asympotic properties of $J_0(\frac{2}{3}\omega)$ we now see that the integral I is uniformly convergent in l in any compact set in $\mathrm{Re}(l)>-\frac{1}{2}$ and in β in $-2+\eta\leqslant\beta\leqslant-\frac{5}{4}-\eta$, $\eta>0$. Accordingly, for any $\epsilon>0$, we can find positive constants δ_1,δ_2,X_1, X_2 independent of l and β such that

$$|I-\int_{x'}^{x''}\int_{y'}^{y''}|x^\beta G(x,y)|^2 dxdy|<\epsilon \tag{A4}$$

for $x'<\delta_1$, $y^1<\delta_2$, $x''>X_1$, $y''>X_2$ and for β in $-2+\eta\leqslant\beta\leqslant-\frac{5}{4}-\eta$, $\eta>0$.

Now $\delta_i(l)$ and $X_i(l)$, $i=1,2$, in (A2) are independent of β. The uniform convergence of I in l for $-2+\eta\leqslant\beta\leqslant-\frac{5}{4}-\eta$, $\eta>0$, implies that $\delta_i(l)=\delta_i$, $X_i(l)=X_i$ in this subinterval and hence for all β in $-2+\eta\leqslant\beta<\frac{1}{4}-\eta$, $\eta>0$. Hence I is uniformly convergent over compact sets in the respective domains of the parameters l and β.

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Melnikov's method and Arnold diffusion for perturbations of integrable Hamiltonian systems [a)]

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We start with an unperturbed system containing a homoclinic orbit and at least two families of periodic orbits associated with action angle coordinates. We use Kolmogorov–Arnold–Moser (KAM) theory to show that some of the resulting tori persist under small perturbations and use a vector of Melnikov integrals to show that, under suitable hypotheses, their stable and unstable manifolds intersect transversely. This transverse intersection is ultimately responsible for Arnold diffusion on each energy surface. The method is applied to a pendulum–oscillator system.

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1. INTRODUCTION

In a previous paper (Holmes and Marsden)[1] we developed a method for proving the existence of Smale horseshoes in two-degree-of-freedom Hamiltonian and nearly Hamiltonian systems. This paper extends those methods to systems with three or more degrees of freedom. We start with an unperturbed system containing a homoclinic orbit and at least two families of periodic orbits associated with action coordinates. We use KAM theory to show that some of the resulting tori persist under small perturbations and use a vector of Melnikov integrals to show that, under suitable hypotheses, their stable and unstable manifolds intersect transverselly. This transverse intersection is ultimately responsible for Arnold diffusion on each energy surface.

Our methods are a generalization of those of Arnold[2] where "Arnold diffusion" was first introduced. The applications are, however, somewhat different and, we believe, of more direct physical interest.

For two-dimensional forced systems, the existence of transverse homoclinic orbits using Melnikov type methods is discussed in Chow, Hale, and Mallet-Paret,[3] Holmes,[4] and Greenspan and Holmes.[5] These methods apply to two-degree-of-freedom Hamiltonian systems through the process of reduction and are discussed in Holmes and Marsden.[1] These methods also apply to certain infinite-dimensional problems with external forcing and damping; see Holmes and Marsen.[6] The purpose of this paper is to extend the Melnikov method to Hamiltonian systems with three or more degrees of freedom where the new phenomenon of Arnold diffusion arises.

The main example treated in this paper is a Hamiltonian system consisting of a pendulum coupled to two oscillators (with amplitude-dependent frequencies). The system is shown to have Arnold diffusion. Using the techniques in our previous paper, one can also show that the Arnold diffusion on a certain energy surface survives suitable positive and negative damping perturbations.

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We shall assume that our coordinates are given in canonical form. However, many interesting problems involving rigid body dynamics are best done in a more general Lie group theoretic context. This situation is discussed in Holmes and Marsden.[7]

2. TRANSVERSAL INTERSECTION OF INVARIANT MANIFOLDS BY MELNIKOV'S METHOD

In this section we are concerned with perturbations of Hamiltonian systems of the form

$$H^0(q,p,x,y) = F(q,p) + G(x,y), \tag{2.1}$$

where (q,p,x,y) are canonical coordinates on a $2(n+1)$-dimensional symplectic manifold P; q and p are real and $x = (x^1,...,x^n)$, $y = (y_1,...,y_n)$. We assume the coordinates are canonical although, in some examples such as the rigid body, this requires modification (Holmes and Marsden[7]). We shall also assume that action-angle coordinates $(\theta_1,...,\theta_n,I_1,...,I_n)$ can be found in a certain region of phase space such that (2.1) takes the form

$$H^0(q,p,\theta,I) = F(q,p) + \sum_{i=1}^{n} G_i(I_i). \tag{2.2}$$

We also assume that $G_i(0)$ and that

$$\Omega_j(I_j) = \frac{\partial G_j}{\partial I_j} > 0 \quad \text{for } I_j > 0. \tag{2.3}$$

The perturbed problem we consider has the form

$$H^\epsilon(q,p,\theta,I) = F(q,p) + \sum_{i=1}^{n} G_i(I_i) + \epsilon H^1(q,p,\theta,I), \tag{2.4}$$

where H^1 is 2π-periodic in $\theta_1,...,\theta_n$. Now we recall how this $(n+1)$-degree-of-freedom system may be reduced to an n-degree-of-freedeom nonautonomous system; the reader should refer to Holmes and Marsden[1] for details.

Choose one of the action coordinates, say I_n. Since $\Omega_n(I_n) > 0$ for $I_n > 0$, we can invert the equation

$$H^\epsilon(q,p,\theta,I) = h \tag{2.5}$$

to obtain

$$I_n = L^\epsilon(q,p,\theta_1,...,\theta_n,I_1,...,I_{n-1};h). \tag{2.6}$$

If we write

$$L^{\epsilon} = L^{0} + \epsilon L^{1} + O(\epsilon^2), \tag{2.7}$$

then a simple computation shows that

$$L^{0}(q,p,I_1,\ldots,I_{n-1};h) = G_n^{-1}\Big(h - F(q,p) - \sum_{j=1}^{n-1} G_j(I_j)\Big) \tag{2.8}$$

and

$$L^{1}(q,p,\theta_1,\ldots,\theta_n,I_1,\ldots,I_{n-1};h) = -\frac{H^{1}(q,p,\theta_1,\ldots,\theta_n,I_1,\ldots,I_{n-1}),L^{0}(q_1,p,I_1,\ldots,I_{n-1};h)}{\Omega_n(L^{0}(q,p,I_1,\ldots,I_{n-1};h))}. \tag{2.9}$$

Changing variables from t to θ_n and writing $(\ )'$ for $(d/d\theta_n)$ $(\ )$, Hamilton's equations for H^{ϵ} become

$$q' = -\frac{\partial L^{\epsilon}}{\partial p}, \quad p' = \frac{\partial L^{\epsilon}}{\partial q},$$
$$\theta_j' = -\frac{\partial L^{\epsilon}}{\partial I_j}, \quad I_j' = -\frac{\partial L^{\epsilon}}{\partial \theta_j}, \quad j = 1,\ldots,n-1. \tag{2.10}$$

Using (2.7)–(2.9), Eqs. (2.10) are in the form of a 2π-periodically forced n-degree-of-freedom Hamiltonian system. Notice that L^{0} is (formally) completely integrable, having n constants of the motion given by

$$L^{0}(\text{energy}) \text{ and } (I_1,\ldots,I_{n-1}) = (l_1,\ldots,l_{n-1}),$$

or alternatively,

$$L^{0} \text{ and } (G_1(I_1),\ldots,G_{n-1}(I_{n-1})) = (h_1,\ldots,h_{n-1}).$$

(This reflects the general fact that complete integrability is preserved by the reduction process).

Assume now that the Hamiltonian F has a homoclinic orbit $(\bar q(t),\bar p(t))$ joining a saddle point (q_0,p_0) to itself. (The case of heteroclinic orbits connecting different saddle points proceeds in the same way.) The Hamiltonian system for L^{0} thus has an $(n-1)$-parameter family of invariant $(n-1)$-dimensional tori $T(h_1,\ldots,h_{n-1})$ given by

$$G_j(I_j) = h_j = \text{const } [\text{i.e., } I_j = l_j = G_j^{-1}(h_j)],$$
$$\theta_j = \Omega_j(l_j\theta_n + \theta_j(0) \ (\text{mod } 2\pi), \quad j = 1,\ldots,n-1, \tag{2.11}$$
$$q = q_0, \quad p = p_0.$$

Correspondingly, the system for F has an n-parameter family of invariant tori $T(h_1,\ldots,h_n)$. Henceforth we write the (phase) constants of integration $\theta_j(0)$ as $\theta_j^0 j = 1,\ldots,n-1,n$.

The torus $T(h_1,\ldots,h_{n-1})$ is connected to itself by the n-dimensional homoclinic manifold

$$G_j(I_j) = h_j,$$
$$\theta_j = \Omega_j(I_j)\theta_n + \theta_j^0, \quad j = 1,\ldots,n-1, \tag{2.12}$$
$$q = \bar q(\theta - \theta_n^0), \quad p = \bar p(\theta - \theta_n^0),$$

where the phase constant θ_n^0 associated with the "reduced" degree of freedom appears explicitly. This manifold consists of the coincident stable and unstable manifolds of the torus $T(h_1,\ldots,h_{n-1})$; i.e.,

$$W^{s}(T(h_1,\ldots,h_{n-1})) = W^{u}(T(h_1,\ldots,h_{n-1}))$$

given by (2.12). See Fig. 1.

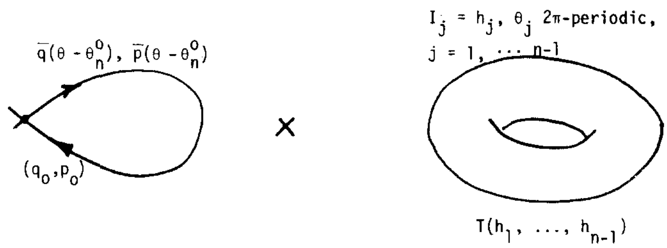

FIG. 1. The homoclinic orbit for the F system $\times$ the invariant torus $T(h_1,\ldots,h_{n-1})$ gives the homoclinic manifold of the torus.

For $\epsilon \neq 0$ the system (2.10) possesses a Poincaré map P_ϵ from (a piece of) $(q,p,\theta_1,\ldots,\theta_{n-1},I_1,\ldots,I_{n-1})$ space to itself, where θ_n goes through an increment of 2π, starting at some fixed value θ_n^0 (which will be suppressed in the notation). The tori $T(h_1,\ldots,h_{n-1})$ are invariant manifolds for P_0. In fact, these tori are isotropic submanifolds (i.e., the canonical 2 form ω vanishes on them), a fact we shall need later.

The program is to show that for $\epsilon \neq 0$ some of the tori persist and that their stable and unstable manifolds intersect transversely. To do this we shall invoke the KAM (Kolmogorov–Arnold–Moser) theory and Melnikov's method. The result will then be interpreted as Arnold diffusion.

Let us first discuss the invariant tori. The manifold obtained by setting $q = q_0, p = p_0$ is a $(2n-2)$-dimensional normally hyperbolic invariant manifold, say M_0, for our Poincaré map P_0. Thus, for ϵ small, M_0 perturbs uniquely to an invariant manifold M_ϵ for P_ϵ. The KAM theory now can be applied to the family of invariant tori $T(h_1,\ldots,h_{n-1})$ on M_0. If the hypotheses of nondegeneracy and nonresonance hold[8] then the torus $T(h_1,\ldots,h_{n-1})$ will perturb to an invariant torus $T_\epsilon(h_1,\ldots,h_{n-1})$ for P_ϵ, for ϵ sufficiently small (depending upon the precise "degree" of nondegeneracy). Moreover, the proof shows that this torus is also isotropic.[9] We note that the perturbed torus T_ϵ has the same frequencies $\Omega_j(h_j)$ as the unperturbed torus and thus the perturbed phase angles do not drift appreciably from the unperturbed ones. We use this fact below.

Although a set of positive measure of the perturbed tori persist near the original ones, the resonant tori containing continuous families of periodic motions generally break into finite sets of alternating elliptic and hyperbolic periodic orbits with associated homoclinic motions, as in Arnold [1978],[8] (p. 397). The boundaries of the elliptic islands are conventionally drawn as homoclinic orbits of a flow: these actually belong to an associated averaged (= canonically transformed) system. Restoration of the terms omitted in averaging leads to the prediction that these islands will, in turn, be surrounded by regions containing transverse homoclinic orbits (cf. Holmes[4]) but these regions are smaller than any power of ϵ, since they can be removed by successive averaging operations. In fact such "stochastic layers" are generally exponentially small in ϵ and attempts to compute them by the Melnikov method necessitate a careful examination of errors. This will be the subject of a further publication; cf. Sanders [1980].[10]

In the case of two degrees of freedom for which the unperturbed reduced system has a hyperbolic saddle point $x_0 = (q_0,p_0)$, solutions of the perturbed system lying in the perturbed stable and unstable manifolds of the perturbed saddle point x_ϵ of the map P_ϵ can be expanded in power series which converge uniformly in the intervals indicated:

$$W^s: \overline{x}^s_\epsilon = \overline{x}(\theta - \theta^0) + \epsilon x^s_1(\theta,\theta^0) + O(\epsilon^2), \quad \theta \in [\theta^0, \infty),$$
$$W^u: \overline{x}^u_\epsilon = \overline{x}(\theta - \theta^0) + \epsilon x^u_1(\theta,\theta^0) + O(\epsilon^2), \quad \theta \in (-\infty, \theta^0], \tag{2.13}$$

where

$$\overline{x}(\theta - \theta^0) = \begin{pmatrix} \overline{q}(\theta - \theta^0) \\ \overline{p}(\theta - \theta^0) \end{pmatrix}$$

is the unperturbed homoclinic orbit. (Recall that the periodic variable θ has replaced time.) For details, see Holmes,[4] Sanders,[10] or Greenspan and Holmes.[5] [Basically (2.13) follows from the fact that the perturbed solutions lie in manifolds of solutions forward- or backward-asymptotic to the perturbed saddle points.] Similarly, solutions lying in the perturbed invariant manifolds $W^s(T_\epsilon), W^u(T_\epsilon)$ of a perturbed torus T_ϵ can be expanded in convergent power series in ϵ in such intervals, since the perturbed actions are ϵ close and the perturbed angles do not drift but remain close to the unperturbed angles on the tori. This result will be used implicitly in what follows.

The perturbed invariant manifolds $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$ of the torus T_ϵ for the map P_ϵ are n-dimensional manifolds lying C^r close to the unperturbed homoclinic manifold given by (2.12), i.e.,

$$F = \bar{h}, \quad I_j = l_j, \quad j = 1,...,n-1, \tag{2.14}$$

where $\bar{h}$ is the energy of the homoclinic orbit for F. Now we are ready to give a criterion for the transversal intersection of $W^s(T_\epsilon)$ *and* $W^u(T_\epsilon)$. In order for the results to be applicable, it is useful to present the hypotheses in terms of data given for the original, rather than the reduced, system.

We consider a Hamiltonian system with $n+1 (\geqslant 3)$ degrees of freedom of the form

$$H^\epsilon(q,p,\theta_1,...,\theta_n,I_1,...,I_n) = F(q,p) + \sum_{i=1}^{n} G_i(I_i) + \epsilon H^1(q,p,\theta_1,...,\theta_n,I_1,...,I_n). \tag{2.15}$$

Introduce the following assumptions and terminology:

(H1) F contains a homoclinic orbit $(\overline{q}(t),\overline{p}(t))$ connecting a saddle point (q_0,p_0) to itself. Let $\bar{h}$ be the energy of this orbit.

(H2) $\Omega_j(I_j) = G'_j(I_j) > 0$ for $j = 1,...,n$.

Let $h > h$ and let the unperturbed homoclinic manifold be filled with an n-parameter family of orbits given by $(\overline{q},\overline{p},\theta_1,...,\theta_n,I_1,...,I_n) = (\overline{q}(t),\overline{p}(t),\Omega_1(I_1)t + \theta^0_1,...,\Omega_n(I_n)t + \theta^0_n, I_1,...,I_n)$. Pick one such orbit and let $\{F,H^1\}$ denote the (q,p) Poisson bracket of $F(q,p)$ and $H^1(q,p,\theta_1,...,\theta_n,I_1,...,I_n)$ evaluated on this orbit. Similarly, let $\{I_k,H^1\} = -\partial H^1/\partial\theta_k, k \equiv 1,...,n-1$ be evaluated on this orbit. Define the *Melnikov Vector* $M(\theta) = (M_1,...,M_{n-1},M_n)$ by

$$M_k(\theta^0_1,...\theta^0_n, h,h_1,h_2,...,h_{n-1}) = \int_{-\infty}^{\infty} \{I_k,H^1\}dt, \quad k = 1,...,n-1$$
$$M_n(\theta^0_1,...,\theta^0_n,h,h_1,h_2,...,h_{n-1}) = \int_{-\infty}^{\infty} \{F,H^1\}dt. \tag{2.16}$$

(We note that $h_n = h - \bar{h} - \sum_{j=1}^{n-1} h_j$; I_n and h_n do not explicitly enter the calculations, since I_n is eliminated by the reduction process; we also note that these integrals need not be absolutely convergent, but we do require conditional convergence.)

(H3) Assume that the constants $G_j(I_j) = h_j, j = 1,...,n$, are chosen so that the unperturbed frequencies $\Omega_1(I_1),...,\Omega_1(I_n)$ satisfy the nondegeneracy conditions [i.e., $\Omega'_j(I_j) \neq 0, j = 1,...,n-1$] and the nonresonance conditions mentioned above (cf. Arnold,[8] Appendix 8).

(H4) Assume that the multiply 2π-periodic Melnikov vector $M: \mathbb{R}^n \rightarrow \mathbb{R}^n$ (which is independent of ϵ) has at least one transversal zero; i.e., there is a point $(\theta^0_1,...,\theta^0_n)$ for which

$$M(\theta^0_1,...,\theta^0_n) = 0$$

but

$$\det[DM(\theta^0_1,...,\theta^0_n)] \neq 0,$$

where DM is the $n \times n$ matrix of partial derivatives of $M_1,...,M_n$ with respect to $\theta^0_1,...,\theta^n_1$, the initial phases of the orbit.

Here is our main theoretical result.

Theorem 2.1: If conditions (H1)–(H4) hold for the system (2.15) then, for ϵ sufficiently small, the perturbed stable and unstable manifolds $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$ of the perturbed torus T_ϵ intersect transversally. (See Fig. 2.)

Remark: The conclusions imply that the perturbed system has no analytic integrals other than the total energy H^ϵ and, for $n+1 \geqslant 3$, that Arnold diffusion occurs. This is dis-

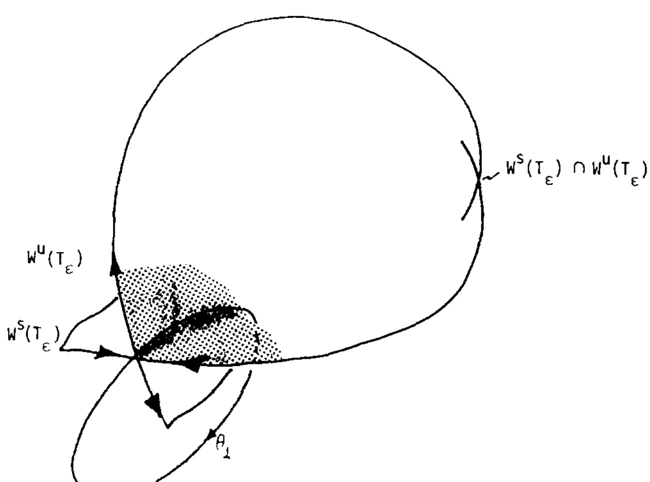

FIG. 2. The stable and unstable manifolds of the invariant torus T_ϵ for the Poincaré map in the reduced space for a system with three degrees of freedom. This figure occurs in (q,p,θ_1,I_1) space [one dimension (I_1) is suppressed], in a θ^0_2 = fixed cross section for fixed total energy h.

cussed in the next section.

Proof: First we notice that the brackets of the original functions project to corresponding brackets of the reduced system:

$$\{L^0, L^1\} = \frac{1}{[\Omega_n(I_n)]^2}\{F, H^1\} \tag{2.17}$$

and

$$\{I_k, L^1\} = -\frac{1}{\Omega_n(I_n)}\{I_k, H^1\}, \quad k = 1,\dots,n-1 \tag{2.18}$$

(see Holmes and Marsden,[1] Prop. 3.1).

We next wish to relate these brackets to a vector measuring the distance between the perturbed stable and unstable manifolds.

Consider the suspended system in $(q,p,\theta_1,\dots,\theta_{n-1},I_1,\dots,I_{n-1})$ space. Pick a transversal Σ_{θ^0} to the unperturbed homoclinic manifold $W^s(T) = W^u(T)$ in $(q,p,\theta_1,\dots,\theta_{n-1},I_1,\dots,I_{n-1})$ space at the point $(\bar{q}(0),\bar{p}(0),\theta_1^0,\dots,\theta_{n-1}^0,I_1,\dots,I_{n-1})$ and at "time" θ_n^0. Now for ϵ sufficiently small, $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$ intersect Σ_{θ^0} in unique points in $(q,p,\theta_1,\dots,\theta_{n-1},I_1,\dots,I_{n-1})$ space, which we denote

$x_\epsilon^s(\theta^0,\theta_n^0)$ and $x_\epsilon^u(\theta^0,\theta_n^0)$.

The unique trajectories in $(q,p,\theta_1,\dots,\theta_{n-1},I_1,\dots,I_{n-1},\theta_n)$ space with these points as initial conditions and time θ_n will be denoted

$x_\epsilon^s(\theta^0,\theta_n)$ and $x_\epsilon^u(\theta^0,\theta_n)$.

As in Holmes and Marsden,[6] a measure of the distance between these vectors and the tangent to $W^s(T) = W^u(T)$ in the "θ_n direction," i.e., the direction of X_{L^0}, the Hamiltonian vector field of the unperturbed dynamics, is provided by the symplectic form ω. Let

$$\Delta_{\epsilon,n}(\theta_n,\theta_n^0) = \omega(X_{L^0}, x_\epsilon^s - x_\epsilon^u) \stackrel{\text{def}}{=} \Delta_{\epsilon,n}^+ - \Delta_{\epsilon,n}^- + O(\epsilon^2).$$

Now as $\theta_n \to +\infty, x_\epsilon^s \to T_\epsilon$ and as $\theta_n \to -\infty, x_\epsilon^u \to T_\epsilon$ so, as in Holmes and Marsden[6] Lemma 5, we obtain

$$\Delta_{\epsilon,n}(\theta_n^0) = \Delta_{\epsilon,n}(\theta_n^0,\theta_n^0) - \frac{\epsilon M_n(\theta_1^0,\dots,\theta_{n-1}^0,\theta_n^0)}{[\Omega(I_n)]^2} + O(\epsilon^2). \tag{2.19}$$

Note that the integrals (2.16) are well defined since one integrates forward along the stable manifold and backward along the unstable manifold [cf. Eq. (2.13)].

A crucial feature of this calculation is the fact that $\Delta_{\epsilon,n}^+(\theta_n,\theta_n^0) \to 0$ as $\theta_n \to \pm\infty$ since ω vanishes identically on T. This holds as follows. The invariant tori are isotropic and $\Delta_{\epsilon,n}^+(\theta_n,\theta_n^0) = \omega(X_{L^0}, \epsilon x_1^s)$ where X_{L^0} and x_1^s are evaluated on the unperturbed homoclinic manifold and x_1^s is the solution of the first variation equation. Since X_{L^0} is tangent to T, x_1^s necessarily approaches a tangent to T, so as T is isotropic, $\Delta_{\epsilon,n}^+ \to 0$. We note that in this context the perturbed torus T_ϵ may move [by $O(\epsilon)$] and need not remain fixed as in the special case treated by Arnold[2] or as in Melnikov's[11] paper (cf. Holmes[4]).

Thus, $M_n(\theta_1^0,\dots,\theta_{n-1}^0,\theta_n^0)$ measures the leading nontrivial component of the distance between $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$ (up to a constant) in a direction transverse to the "dynamic" variable θ_n. Likewise, $M_i (i = 1,\dots,n-1)$ measures the distance between $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$ in the direction transverse to the generator of the θ_i variable. The theorem now follows from these facts.

Remarks: 1. One can, of course, permute which of the action-angle variables is used for the reduction procedure. The remaining oscillators must satisfy the KAM nonresonance and nondegeneracy conditions.

2. Gruendler[12] has treated the $2n$-dimensional, periodically forced case in which one also has an n-parameter family of unperturbed homoclinic orbits but in which they are homoclinic orbits to a hyperbolic saddle *point* x and $\dim W^s(x) = \dim W^u(x) = n$. Again one obtains a generalized n vector of Melnikov functions each depending upon n arguments, one of which is the section time (θ_n^0) and the remaining $n-1$ of which serve to parametrize the family of orbits. The manifolds $W^s(x)$ and $W^u(x)$ are both necessarily isotropic, so one can proceed in a way analogous to that here. However, no KAM theory is needed and ordinary horseshoes rather than Arnold diffusion occur. Gruendler applies the theory to the case of a periodically forced spherical pendulum.

3. The theorem can be somewhat generalized. For example, many integrable systems do not decompose precisely as assumed in the form $F(q,p) + \Sigma_{j=1}^n G_j(I_j)$ and one sometimes finds that the unperturbed "frequencies, " $\Omega_j = \partial G_j/\partial I_j$, also depend upon (q,p). If this occurs, and $\Omega_j(I_j,q,p)$ is not constant on the unperturbed manifold, then it must be incorporated into the Poisson brackets [cf. Eqs. (2.17) and (2.18)]. This situation will be dealt with in Holmes and Marsden.[7]

4. Alan Weinstein has pointed out that even without hypothesis (H4), the stable and unstable manifolds of the perturbed torus T_ϵ must intersect. This comes about as follows. As in the standard Melnikov analysis (Holmes and Marsden),[6] pick a $2n$-dimensional cross section $\Sigma_{\theta_n^0}$. The stable and unstable manifolds T_ϵ for the associated Poincaré map, $W^s(T_\epsilon)$ and $W^u(T_\epsilon)$, are Lagrangian submanifolds of $\Sigma_{\theta_n^0}$ which are coincident at $\epsilon = 0$. Lagrangian intersection theory (Arnold[13] and Weinstein[14]) shows that the perturbed manifolds must intersect. This observation generalizes one of McGehee and Meyer.[15] It follows that the *hypothesis* $(H4)$ *holds for generic perturbation terms* H^1. However, condition (H4) allows one to check transversality in *specific cases*.

5. In contrast to our results, Easton and McGehee[16] use Moser's[17] fixed point theorem to show that some homoclinic orbits in a model system survive under special perturbations. Alan Weinstein points out that, similarly, at least two homoclinic orbits survive perturbations of the spherical pendulum's S^1 family of homoclinic orbits.

3. NONINTEGRABILITY AND ARNOLD DIFFUSION

If the stable and unstable manifolds $W^s(\Lambda), W^u(\Lambda)$ of a hyperbolic invariant set Λ intersect transversely then it follows from the lambda lemma (Palis,[18] Newhouse[19]) that $W^s(\Lambda)$ accumulates on itself and $W^u(\Lambda)$ accumulates on itself. A similar result holds for the invariant tori in the present case (cf. Arnold,[2] Theorem 1); more precisely, if $\Delta_1 \subset W^u(T_\epsilon)$ is an n-dimensional neighborhood of a transverse homoclinic point $x \in W^u(T_\epsilon) \cap W^s(T_\epsilon)$, and $\Delta_2 \subset W^u(T_\epsilon)$ is any open disk, then there are points of $\bigcup_{n>0} P_\epsilon^n(\Delta_1)$ lying arbitrarily close to Δ_2. Such a torus T_ϵ is said to be a *transition torus*. The torus is said to lie in a *transition chain* of transition tori $T_\epsilon^1, T_\epsilon^2, \ldots, T_\epsilon^k$ if the unstable manifold $W^u(T_\epsilon^j)$ of the jth torus transversely intersects the stable manifold of the $(j+1)$st. This holds in our case since, by KAM theory, the set of "sufficiently irrational" tori preserved when $\epsilon \neq 0$ has measure $\mu(\epsilon) \to 1$ as $\epsilon \to 0$ (it is, in fact, a Cantor set). Thus, for sufficiently small ϵ one can find tori $T_\epsilon^j, T_\epsilon^{j+1}$ which are, along with their stable and unstable manifolds, arbitrarily C^r close away from the torus and these manifolds have large "oscillations" near the torus as in Holmes and Marsden,[1] Fig. B.1. It follows that if $W^u(T_\epsilon^j)$ intersects $W^s(T_\epsilon^j)$ transversely it must also intersect $W^s(T_\epsilon^{j+1})$ transversely. Applying the same argument to $T_\epsilon^{j+1}, T_\epsilon^{j+2}, \ldots$, one constructs a transition chain. Orbits lying in $W^u(T_\epsilon^j)$ therefore accumulate on $W^u(T_\epsilon^k)$ for $k \geqslant j$ and these orbits and nearby ones provide a mechanism by which solutions can "diffuse" from the neighborhood of the torus to any other in the transition chain. (cf. Arnold,[2] Theorem 2). An argument analogous to that above shows that $W^u(T_\epsilon^{j+1})$ intersects $W^s(T_\epsilon^j)$ and thus that diffusion can take place in both directions along the chain. Note, however, that the length of the chain is generally governed by the perturbation strength ϵ, since as ϵ increases the set of perturbed tori generally diminishes.

The mechanism outlined above, which we attempt to portray in Fig. 3, is the basis for Arnold diffusion. Clearly it can only occur in systems with three or more degrees of freedom ($n \geqslant 2$), since the unperturbed $2n$-dimensional reduced Poincaré map must admit continuous families of tori connected by smooth homoclinic manifolds, and this cannot occur in two dimensions. For more information, numerical examples, and physical insights, see Chirikov[20] and Lieberman.[21] The main physical consequence of diffusion is that (given sufficient time) energy can be transferred back and forth in relatively large amounts between distinct physical

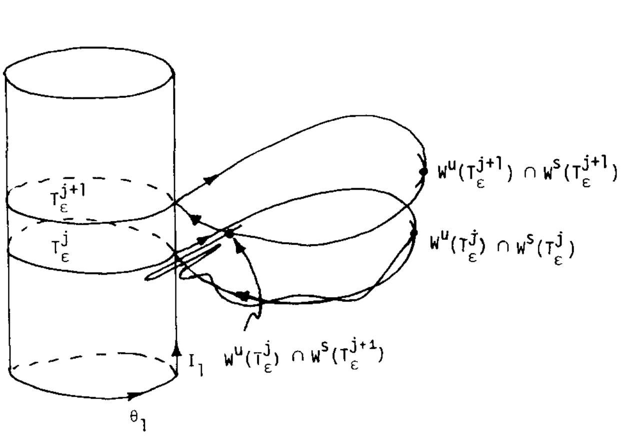

FIG. 3. Intersections of manifolds and Arnold diffusion in a three degree of freedom system. The Poincaré section $\theta_2 = \theta_2^0$ is shown on the energy surface $H^\epsilon = h$.

components or vibration modes of the system. Moreover this transfer of energy will typically take place in an irregular manner, in contrast to the regular quasiperiodic energy transfer occuring between modes in linear or other integrable systems.

Thus, in contrast to the two-degree-of-freedom case, in which the sufficiently irrational invariant tori, preserved for small perturbations, serve as boundaries to regions of homoclinic (chaotic) motions in the three-dimensional total-energy manifold, in systems with three or more degrees of freedom the solutions can diffuse from torus to torus along transition chains; the n tori which are preserved do not bound regions of $2n+1$ space for $n \geqslant 2$. In our case, since two-way transition chains can be chosen, we can find periodic motions of arbitrarily high period close to such chains, just as in the standard two-dimensional horseshoe example. The density of the set of such motions and the dense orbit accompanying them guarantees nonexistence of any additional analytic integrals other than the total energy H^ϵ. (In fact one sees that such dense orbits exist within neighborhoods of any transverse homoclinic orbits connecting a torus to itself, without invoking the idea of diffusion.)

The presence of a small amount of noise in a system is believed to "stabilize" in some sense the occurrence of Arnold diffusion, in the same way that noise often "stabilizes" or "makes visible" horseshoes (cf. Holmes and Marsden.[1]).

4. AN EXAMPLE:THE SIMPLE PENDULUM COUPLED TO TWO OSCILLATORS

We illustrate the theory developed above with a generalization of our earlier two-degree-of-freedom pendulum–oscillator model (Holmes and Marsden [1981][1]). Consider a simple pendulum linearly coupled to two nonlinear oscillators. For simplicity we assume that the oscillators are identical (this is not important) and that their Hamiltonians can be expressed as $G((x_i^2 + y_i^2)/2)$ or, equivalently, in action-angle coordinates as

$$G(I_i), \quad i = 1,2, \tag{4.1}$$

with

$$\Omega(I_i) = \frac{\partial G}{\partial I_i}(I_i) \neq 0 \quad \text{for } I_i > 0 \tag{4.2a}$$

and

$$\Omega'(I_i) = \frac{\partial^2 G}{\partial I_i^2}(I_i) \neq 0 \tag{4.2b}$$

[cf. Eqs. (2.3) and condition (H2) of Sec. 2]. Elimination of either I_1 or I_2 by reduction is then possible. For definiteness, we shall assume that I_2 is removed. Our assumption of the form $G((x_i^2 + y_i^2)/2)$ is merely for computational convenience, since more "realistic" anharmonic oscillators lead to Hamiltonians $G(I_i)$ expressed in terms of, for example, elliptic functions (cf. Greenspan and Holmes[5]).

The system to be studied has the Hamiltonian

$$H^\epsilon = p^2/2 - \cos q + G_1(I_1) + G(I_2) + (\epsilon/2)[((2I_1)^{1/2}\sin\theta_1 - q)^2 + ((2I_2)^{1/2}\sin\theta_2 - q)^2]. \tag{4.3}$$

The unperturbed orbits in the homoclinic manifold are given by

$$(\bar{q}, \bar{p}, \theta_1, \theta_2, I_1, I_2) = (\pm 2 \arctan(\sinh t), \pm 2 \operatorname{sech} t, \Omega(l_1)t + \theta_1^0, \Omega(l_2)t + \theta_2^0, l_1, l_2), \quad (4.4)$$

where $h > 1$ is the total energy and $\bar{h} = 1$ the energy of the homoclinic orbit, and $G_1(l_1) = h_1, G_2(l_2) = h - 1 - h_1$. Assumptions H(1) and H(2) of Theorem 3.1 are therefore satisfied and, in view of (4.2a) and (4.2b) we can pick h and h_1 so that the nonresonance conditions necessary for application of the KAM theorem are met. To check the final assumption we compute the Poisson brackets $\{I_1, H^1\}$ and $\{F, H^1\}$. From (4.3) we have

$$\{I_1, H^1\} = -\frac{\partial H^1}{\partial \theta_1} = -((2I_1)^{1/2} \sin \theta_1 - q)(2I_1)^{1/2} \cos \theta_1$$

and

$$\begin{aligned}\{F, H^1\} &= \frac{\partial F}{\partial q}\frac{\partial H^1}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial H^1}{\partial p} \\ &= \sin q \cdot 0 - p[-((2I_1)^{1/2} \sin \theta_1 - q_1) \\ &\quad - ((2I_2)^{1/2} \sin \theta_2 - q)] \qquad (4.5) \\ &= p[(2I_1)^{1/2} \sin \theta_1 + (2I_2) \sin \theta_2 - 2q].\end{aligned}$$

Thus, using (4.4) we have

$$\begin{aligned}M_1(\theta_1^0, \theta_2^0, h, h_1) &= \int_{-\infty}^{\infty} -[(2l_1)^{1/2} \sin(\Omega(l_1)t + \theta_1^0) \\ &\quad \mp 2 \arctan(\sinh t)] \\ &\quad \times (2l_1)^{1/2} \cos(\Omega(l_1)t + \theta_1^0) dt\end{aligned}$$

and

$$\begin{aligned}M_2(\theta_1^0, \theta_2^0, h, h_1) &= \int_{-\infty}^{\infty} \pm 2 \operatorname{sech} t\, [(2l_1)^{1/2} \sin(\Omega(l_1)t + \theta_1^0) \\ &\quad + (2l_2)^{1/2} \sin(\Omega(l_2)t + \theta_2^0) \mp 4 \arctan(\sinh t)] dt. \qquad (4.6)\end{aligned}$$

Noting that the integrals of products of odd and even functions vanish over the infinite domain and taking the positive branch of the homoclinic manifold, these two functions become

$$\begin{aligned}M_1 &= 2(2l_1)^{1/2}\left[\int_{-\infty}^{\infty} \arctan(\sinh t) \sin(\Omega(l_1)t) dt\right] \sin \theta_1^0, \\ M_2 &= 2(2l_1)^{1/2}\left[\int_{-\infty}^{\infty} \operatorname{sech} t \cos(\Omega(l_1)t) dt\right] \sin \theta_1^0 \\ &\quad + 2(2l_2)^{1/2}\left[\int_{-\infty}^{\infty} \operatorname{sech} t \cos(\Omega(l_2)t) dt\right] \sin \theta_2^0. \qquad (4.7)\end{aligned}$$

For brevity we write

$$\Omega(l_1) = \omega_1, \quad \Omega(l_2) = \omega_2. \qquad (4.8)$$

To evaluate the first conditionally convergent integral we choose, for computational convergence, the limits as follows:

$$\begin{aligned}&\lim_{N\to\infty} \int_{-N\pi/\omega_1}^{N\pi/\omega_1} \arctan(\sinh t) \sin \omega_1 t\, dt \\ &= \lim_{N\to\infty}\left\{ -\frac{1}{\omega_1} \arctan(\sinh t) \cos\omega_1 t \Big|_{-N\pi/\omega_1}^{N\pi/\omega_1} + \frac{1}{\omega_1}\int_{-N\pi/\omega_1}^{N\pi/\omega_1} \frac{\cos \omega_1 t}{1 + \sinh^2 t} dt\right\} \\ &= \frac{1}{\omega_1}\int_{-\infty}^{\infty} \operatorname{sech}^2 t \cos \omega_1 t\, dt \\ &= \frac{1}{\omega_1}(\pi\omega_1) \operatorname{csch}\left(\frac{\pi\omega_1}{2}\right). \qquad (4.9)\end{aligned}$$

The final integral is obtained by the method of residues. Similarly, we have

$$\int_{-\infty}^{\infty} \operatorname{sech} t \cos \omega_j t\, dt = \pi\omega_j \operatorname{sech}\left(\frac{\pi\omega_j}{2}\right), \quad j = 1,2, \qquad (4.10)$$

and thus

$$\begin{aligned}M_1 &= 2\pi(2l_1)^{1/2} \operatorname{csch}\left(\frac{\pi\omega_1}{2}\right) \sin \theta_1^0, \\ M_2 &= \left[(2l_1)^{1/2}\omega_1 \operatorname{sech}\left(\frac{\pi\omega_1}{2}\right) \sin \theta_1^0 \right. \\ &\quad \left. + (2l_2)^{1/2}\omega_2 \operatorname{sech}\left(\frac{\pi\omega_2}{2}\right) \sin \theta_2^0\right]. \qquad (4.11)\end{aligned}$$

One obtains a similar result (with an appropriate change of sign) on the negative branch of the manifold.

We therefore find zeroes when $\theta_1^0 = k\pi, \theta_2^0 = l\pi$ for all integers l,k and it is easy to check that

$$\det DM = \frac{\partial M_1}{\partial \theta_1^0}\frac{\partial M_2}{\partial \theta_2^0} - \frac{\partial M_1}{\partial \theta_2^0}\frac{\partial M_2}{\partial \theta_1^0}\Big|_{\substack{\theta_1^0 = k\pi \\ \theta_2^0 = l\pi}}$$

$$\pm 8\pi^2\omega_2(l_1 l_2)^{1/2} \operatorname{csch}\left(\frac{\pi\omega_1}{2}\right)\operatorname{sech}\left(\frac{\pi\omega_2}{2}\right) \neq 0. \qquad (4.12)$$

Thus the final assumption is satisfied for suitable choices of h and h_1 and we have

Theorem 4.1: For ϵ sufficiently small the Hamiltonian system (4.3) has a set of two-dimensional invariant tori of positive measure each of whose unstable manifolds intersects its stable manifold transversely. Moreover, a finite transition chain of such tori $T_\epsilon^1, ..., T_\epsilon^m$ can be chosen such that $W^u(T_\epsilon^j)$ intersects $W^s(T_\epsilon^{j+1})$ transversely and $W^u(T_\epsilon^{j+1})$ intersects $W^s(T_\epsilon^j)$ transversely, $j = 1, ..., m - 1$. Thus, orbits can be found which pass from the neighborhood of any torus T_ϵ^k to the neighborhood of any other torus T_ϵ^l in the chain. This situation obtains on every energy level $H^\epsilon = h > 1$.

Remarks: 1. Arnold's[2] example is similar to ours in some respects, but he employed explicit external forcing, taking a t-periodic two-degree-of-freedom system $H^\epsilon(q,p,\theta,I,t)$ rather than a three-degree-of-freedom autonomous system. This perturbation was further chosen to vanish on the tori, so that the perturbed tori lie in the same positions as the unperturbed tori. As we remarked in Sec. 3, this is not necessary since the bracket $\omega(X_{L_0}, X_{L_1}) = \{L^0, L^1\}$ vanishes on the unperturbed isotropic tori, and thus the integral of the Poisson bracket along the unperturbed orbits still provides a good measure of the separation of the perturbed manifolds.

2. Although the theorem asserts that diffusion occurs on *every* energy level $h > 1$, the latitude available for choice of h_1 and hence for satisfaction of the nonresonance conditions increases with h. Thus the "sufficiently small ϵ" approaches zero as $h \rightarrow 1$.

5. CONCLUSIONS

This paper and its companions (Holmes and Marsden[1,7]), address the general question of perturbations of integrable multidimensional Hamiltonian systems. A particular area of interest is the development of a method for investigating the integrability of the perturbed problem, and for providing a qualitative description of orbits in phase space.

In the present paper we have combined a reduction technique with a vectorial version of Melnikov's[11] method to establish the existence of Arnold diffusion in Hamiltonian systems with at least three degrees of freedom. This in turn implies that the system is nonintegrable in the classical sense: there are no analytic integrals other than the total energy. The method is applied to the specific case of a pendulum coupled to two nonlinear oscillators. It is shown that the stable and unstable manifolds of nonresonant tori that survive under a small perturbation intersect transversely. We briefly discuss how this enables points in phase space to diffuse.

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Global theorems for boundary-free viscous incompressible fluid flows of finite energy [a)]

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It is shown that the *action* for boundary-free incompressible fluid flow (i.e., the time-integral of the kinetic energy of the motion) is an absolute minimum with respect to all velocity-field transformations $\mathbf{u}\to\mathbf{u}^*$ if $\mathbf{u}^*$ is structured suitably in terms of $\mathbf{u}$ and an arbitrary solenoidal test field $\mathbf{f}$. As suggested by this physical minimum principle, inequality analysis is applied to obtain an upper bound on the time derivative of the dissipation integral, from which there follow sufficient conditions for a monotone-decreasing dissipation integral and a monotone-decreasing global Reynolds number. The latter result provides an experimentally consistent necessary condition for passage from laminar to turbulent flow. Finally, inequality analysis is employed to derive a time-dependent lower bound on the maximum velocity gradient in a generic boundary-free flow of finite energy.

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I. INTRODUCTION

There does not exist[1–5] an exclusively $\mathbf{u}$-dependent functional which is stationary in the function-space neighborhood of any solution to the Navier–Stokes equation

$$\partial\mathbf{u}/\partial t + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u} + \rho^{-1}\nabla p = 0, \quad \nabla\cdot\mathbf{u}\equiv 0. \tag{1}$$

In (1), $\mathbf{u} = \mathbf{u}(\mathbf{x},t)$ denotes the velocity field of an incompressible viscous fluid, $p = p(\mathbf{x},t)$ is the fluid pressure, and ν and ρ are the constant kinematic viscosity and constant density of the fluid, respectively. Although a conventional variational principle for (1) cannot be formulated, it is possible to set up an adjoint-field variational principle[6] by introducing an unphysical auxiliary solenoidal flow; however, since the auxiliary flow must vanish identically as a consequence of the adjoint-field variational principle, the practical usefulness of such a variational principle is known to be quite limited.[6]

A physical *minimum principle* for viscous incompressible boundary-free flows of finite energy is presented in Sec. II. It is shown in (11) that the *action* defined by (10), the time integral of the kinetic energy of the motion, is an absolute minimum with respect of all velocity-field transformations $\mathbf{u}\to\mathbf{u}^*$ provided that $\mathbf{u}$ satisfies (1) and $\mathbf{u}^*$ is structured according to (8), where $\mathbf{f}$ is an arbitrary solenoidal test field.

In Sec. III inequality analysis suggested by the minimum principle is applied to obtain the upper bound (18) on the inertial-force viscous-force inner-product integral defined by (7). The result (18) is then used to establish sufficient conditions for a monotone-decreasing dissipation integral (4) and a monotone-decreasing global Reynolds number (14). The latter result provides the experimentally consistent necessary condition for passage from laminar to turbulent flow: $R > 4.410$.

In Sec. IV it is shown that the inner-product integral (7) also has the bound displayed in (33). From this result there follows the time-dependent lower bound on the maximum velocity gradient that is exhibited in (35).

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These global theorems for boundary-free Navier–Stokes incompressible fluid flow are valid quite generally, irrespective of the velocity-field's initial value, for all flows such that the energy integral (2) is finite at the initial instant of time. This assumption requires the flow velocity to vanish as $|\mathbf{x}|\to\infty$, but it does not restrict the flow for finite values of $\mathbf{x}$.

II. PHYSICAL MINIMUM PRINCIPLE

Consider boundary-free flows of finite kinetic energy $\frac{1}{2}\rho A$, where

$$A = A(t) \equiv \int |\mathbf{u}|^2\, d^3x, \tag{2}$$

with the integration over all $\mathbf{x}$ in unbounded three-dimensional Euclidean space R_3. Since $|\mathbf{u}|$ can be assumed to be bounded for all $\mathbf{x}$ and t, the finiteness of (2) is guaranteed by the condition $\lim_{|\mathbf{x}|\to\infty}(|\mathbf{x}|^{3/2}|\mathbf{u}|) = 0$. Notice that (2) is a Liapunov functional,

$$\dot{A} \equiv dA/dt = -2\nu A_1, \tag{3}$$

$$A_1 = A_1(t) \equiv -\int (\mathbf{u}\cdot\nabla^2\mathbf{u})\, d^3x = \int |\nabla\mathbf{u}|^2\, d^3x\ (>0), \tag{4}$$

as a consequence of (1) and Gauss' theorem, where $|\nabla\mathbf{u}|^2 \equiv (\partial u_i/\partial x_j)(\partial u_i/\partial x_j)$. However, the dissipation integral A_1 may increase or decrease with time, since it also follows from (1) and Gauss' theorem that

$$\dot{A}_1 \equiv dA_1/dt = -2\nu A_2 + 2I, \tag{5}$$

where

$$A_2 = A_2(t) \equiv \int |\nabla^2\mathbf{u}|^2\, d^3x\ (>0), \tag{6}$$

$$I = I(t) \equiv \int (\mathbf{u}\cdot\nabla\mathbf{u})\cdot(\nabla^2\mathbf{u})\, d^3x. \tag{7}$$

The inertial-force viscous-force inner-product integral defined by (7) is usually positive and may be dominantly so in (5), as in a transition from smooth laminar flow to rapidly varying turbulent flow, with A_1 typically increasing during

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the transition by several orders of magnitude.

Let $\mathbf{f} = \mathbf{f}(\mathbf{x},t)$ denote an arbitrary solenoidal test field[7] in $R_3 \times (t',t'')$. Infinitely differentiable and nonzero over a compact point set contained in the interior of $R_3 \times (t',t'')$, $\mathbf{f}$ vanishes identically along with all of its derivative at the terminal times $t = t',t''$. Define the transformed flow

$$\mathbf{u}^* \equiv \mathbf{u} + \partial \mathbf{f}/\partial t + \nu \nabla^2 \mathbf{f} + \mathbf{u}\cdot\nabla \mathbf{f} - \mathbf{f}\cdot\nabla \mathbf{u}. \tag{8}$$

From the solenoidal quality of $\mathbf{u}$ and $\mathbf{f}$ it follows that (8) is solenoidal: $\nabla\cdot\mathbf{u}^* \equiv 0$. Moreover, $\mathbf{u}^* = \mathbf{u}$ at $t = t',t''$ because $\mathbf{f}$ and its derivatives vanish at $t = t',t''$. Observe, however, that the transformed flow (8) is not required to satisfy (1); rather, what makes (8) significant is that $(\mathbf{u}^* - \mathbf{u})$ is generally orthogonal to $\mathbf{u}$ in the Hilbert-space sense,

$$\int_{t'}^{t''} \int (\mathbf{u}^* - \mathbf{u})\cdot\mathbf{u}\, d^3x\, dt = 0, \tag{9}$$

since $\mathbf{u}$ satisfies (1) throughout $R_3 \times (t',t'')$. Hence, the *action*

$$W = W[\mathbf{u}] \equiv \frac{\rho}{2} \int_{t'}^{t''} A\, dt \tag{10}$$

is an absolute minimum with respect to all flow changes $\mathbf{u} \to \mathbf{u}^*$,

$$\begin{aligned} W^* \equiv W[\mathbf{u}^*] &= \frac{\rho}{2} \int_{t'}^{t''} \int |\mathbf{u}^*|^2\, d^3x\, dt \\ &= W[\mathbf{u}] + W[\mathbf{u}^* - \mathbf{u}] \\ &\Rightarrow W < W^*. \end{aligned} \tag{11}$$

Conversely, the minimum principle (11) for arbitrary $\mathbf{u}^*$ defined according to (8) implies that $\mathbf{u}$ satisfies (1) through $R_3 \times (t',t'')$.[8] The case of strict inequality holds in (11) because a test field $\mathbf{f}(\not\equiv 0)$ cannot satisfy the linear homogeneous backward diffusion equation which follows from (8) and $\mathbf{u}^* \equiv \mathbf{u}$ through $R_3 \times (t',t'')$.

Noether's analysis can be applied to derive global dynamical relations from (11), just as if (11) were a variational principle with $\mathbf{u}^*$ unstructured and close to $\mathbf{u}$ in a function-space sense. Thus, for example, (3) is obtained by prescribing a sequence of test field such that $\mathbf{f} \doteq \phi(t)\mathbf{u}$, $(\phi(t') = \phi(t'') = 0)$, substituting $\mathbf{u}^* \doteq (1 + \dot\phi)\mathbf{u} + \phi(\partial \mathbf{u}/\partial t + \nu\nabla^2 \mathbf{u})$ into (11), and taking ϕ to be small. Similarly, (5) is obtained by prescribing $\mathbf{f} \doteq \psi(t)\nabla^2\mathbf{u}$, $(\psi(t') = \psi(t'') = 0)$, and substituting the associated $\mathbf{u}^*$ given by (8) into (11).

The functional (10) can be recast in a form that relates to the results in the following sections. Since $\mathbf{u}$ in (10) must satisfy (1), use can be made of (3) and (5) after performing two integrations by parts with respect to t, and (10) becomes

$$W = \frac{\rho}{2}(tA + \nu t^2 A_1)\Big|_{t'}^{t''} + \rho\nu \int_{t'}^{t''} t^2(\nu A_2 - I)dt. \tag{12}$$

Evaluated at the terminal times t' and t'', the lead terms in (12) are invariant under the replacement $\mathbf{u} \to \mathbf{u}^*$, because $\mathbf{u}^* = \mathbf{u}$ at $t = t',t''$. On the other hand, the entire right-hand side of (12) must increase under the replacement $\mathbf{u} \to \mathbf{u}^*$, in accord with (11). Hence, the quantity $(\nu A_2 - I)$ is minimal for $\mathbf{u}$ satisfying (1) in the context of $\mathbf{u} \to \mathbf{u}^*$ flow transformations. This observation suggests that useful dynamical formulas can be obtained by applying inequality analysis to (7) and (5), as is done in the following sections.

III. MONOTONE-DECREASING DISSIPATION INTEGRAL AND GLOBAL REYNOLDS NUMBER

There are two dimensionless variables associated with the integral quantities (2), (4), and (6). First, we have the *broadness*[9] of the velocity field

$$B = B(t) \equiv A A_1^{-2} A_2 - 1. \tag{13}$$

The latter quantity is positive, because the Schwarz inequality guarantees that $B \geqslant 0$ and the critical case $B = 0$ (requiring a Boussinesq $\nabla^2\mathbf{u} = -A^{-1}A_1\mathbf{u}$ flow of infinite energy in R_3) is precluded. In the case of freely decaying isotropic homogeneous turbulence through a finite spatial region, B is quasiconstant with time, changing only slowly from one period of decay to the next.[9]

The second dimensionless variable is the *global Reynolds number*

$$R = R(t) \equiv (AA_1)^{1/4}/\nu, \tag{14}$$

with the composition implied by (2) and (4) of an average flow velocity times an average flow length-extension divided by the kinematic viscosity constant ν. If the flow is smoothly laminar and the quantity (14) is sufficiently small at a certain instant of time, then the flow remains smoothly laminar with a monotone-decreasing dissipation integral (4) for all subsequent time, i.e., there can be no transition to turbulence. In fact, we can establish the following

Theorem 1: If R is less than or equal to 3.902 at any instant of time, then $\dot R < 0$ and $\dot A_1 < 0$ for all subsequent time.

The global Reynolds number (14) is actually monotone decreasing for somewhat larger initial values, and we can also establish

Theorem 2: If R is less than or equal to 4.410 at any instant of time, then $\dot R < 0$ for all subsequent time.

As preliminary to the proofs of these two theorems, note that

$$\begin{aligned} \int (\mathbf{u}\cdot\nabla\mathbf{u})\cdot\mathbf{u}\, d^3x &= \frac{1}{2}\int \mathbf{u}\cdot\nabla|\mathbf{u}|^2\, d^3x \\ &= -\frac{1}{2}\int (\nabla\cdot\mathbf{u})|\mathbf{u}|^2\, d^3x = 0 \end{aligned} \tag{15}$$

by virtue of the incompressibility condition in (1). With the aid of (15), Eq. (7) can be rewritten slightly and bounded from above by applying the Schwarz inequality:

$$\begin{aligned} I &= \int (\mathbf{u}\cdot\nabla\mathbf{u})\cdot(\nabla^2\mathbf{u} + A^{-1}A_1\mathbf{u})\, d^3x \\ &\leqslant \left[\int |\mathbf{u}\cdot\nabla\mathbf{u}|^2\, d^3x \int |\nabla^2\mathbf{u} + A^{-1}A_1\mathbf{u}|^2\, d^3x\right]^{1/2} \\ &< [(|\mathbf{u}|^2_{\max} A_1)(BA^{-1}A_1^2)]^{1/2} \\ &= |\mathbf{u}|_{\max} B^{1/2} A^{-1/2} A_1^{3/2}. \end{aligned} \tag{16}$$

Here $|\mathbf{u}|_{\max} \equiv \max_{\mathbf{x}} |\mathbf{u}(\mathbf{x},t)|$ is the maximum magnitude of the velocity in the flow at the time t, and $|\mathbf{u}\cdot\nabla\mathbf{u}|^2 = u_i u_k(\partial u_j/\partial x_i)(\partial u_j/\partial x_k) \leqslant |\mathbf{u}|^2_{\max}(\partial u_j/\partial x_m)(\partial u_j/\partial x_m)$ has been used in (16), along with definitions (2), (4), (6), and (13). By employing the bound[10]

$$\begin{aligned} |\mathbf{u}|_{\max} &< (2/3(3)^{1/2}\pi)^{1/2} A^{1/8} A_2^{3/8} \\ &= (0.3500)(B+1)^{3/8} A^{-1/4} A_1^{3/4}, \end{aligned} \tag{17}$$

the final member of (16) yields

$$I < (0.3500) B^{1/2}(B+1)^{3/8} A^{-3/4} A_1^{9/4}. \tag{18}$$

In view of (18), one obtains the differential inequality from (5)

$$\frac{1}{2}\dot{A}_1 < -\nu(B+1)A^{-1}A_1^2 + (0.3500)B^{1/2}(B+1)^{3/8}A^{-3/4}A_1^{9/4} = -\nu A^{-1}A_1^2[B+1-(0.3500)B^{1/2}(B+1)^{3/8}R], \quad (19)$$

where (13) and (14) have been introduced. The square-bracketed quantity is nonnegative in the final member of (19) if

$$R \leqslant (2.857)(B+1)^{5/8}B^{-1/2}. \quad (20)$$

Since the minimum value of the right-hand side of (20) is 3.906 (at $B=4$) $\dot{A}_1<0$ is implied by (19) for $R \leqslant 3.906$, irrespective of the value of B. That the latter condition on R is maintained dynamically is seen from the differential inequality for the time rate-of-change of (14), expressed with the aid of (3) and (19) as

$$\dot{R} \equiv dR/dt = \frac{1}{4\nu}(A^{-3/4}\dot{A}A_1^{1/4} + A^{1/4}A_1^{-3/4}\dot{A}_1) < -\frac{1}{2}A^{-3/4}A_1^{5/4}[B+2-(0.3500)B^{1/2}(B+1)^{3/8}R]. \quad (21)$$

Hence, R decreases with time if

$$R \leqslant (2.857)(B+2)B^{-1/2}(B+1)^{-3/8}. \quad (22)$$

Irrespective of the value of B, (22) is satisfied for $R \leqslant 4.410$, since the minimum value of the right-hand side of (22) is 4.410 (at $B=10.70$). This completes the demonstration of Theorems 1 and 2. ■

Because a rapid increase in R is concomitant with a transition from laminar to turbulent flow, Theorem 2 indicates that $R>4.410$ is a necessary condition for the initiation of turbulence. For freely decaying isotropic homogeneous turbulence through a finite spatial region of volume V with $|\mathbf{u}|$ rapidly approaching zero outside the region, the quantity (7) is given by[9]

$$I = \langle(\mathbf{u}\cdot\nabla\mathbf{u})\cdot(\nabla^2\mathbf{u})\rangle V$$
$$= B(\tfrac{2}{3} + (0.090045)\ln B)\nu A^{-1}A_1^2, \quad (23)$$

where $A = \langle|\mathbf{u}|^2\rangle V$ and $A_1 = \langle|\nabla\mathbf{u}|^2\rangle V$. One obtains

$$R > B^{1/2}(B+1)^{-3/8}(1.905 + 0.2573\ln B) \quad (24)$$

by substituting (23) into the left-hand side of (18). Increasing monotonically with increasing B, the right-hand side of (24) attains the value 4.406 for $B=37.0$, the largest *broadness* observed for isotropic homogeneous turbulence.[9] Thus, the necessary condition for turbulence, $R>4.410$, agrees with experiment.

IV. LOWER BOUND ON THE MAXIMUM VELOCITY GRADIENT

Manifesting the effect of inertial-force nonlinearity in (5), the inner-product integral (7) admits a supplementary upper bound which can be employed in place of (18) in analytical applications. The latter inequality, displayed below in (33), provides an immediate lower bound on the maximum velocity gradient at time t. Large values of the velocity gradient are characteristically featured by the "solutions turbulente" of Leray and more recent authors,[11] and thus (35) can serve to indicate the presence of (possible local) turbulence in the flow.

First observe that

$$\int (\partial u_i/\partial x_k)u_j(\partial^2 u_i/\partial x_j\partial x_k)\,d^3x$$
$$= -\frac{1}{2}\int (\partial u_j/\partial x_j)(\partial u_i/\partial x_k)(\partial u_i/\partial x_k)\,d^3x$$
$$=0 \quad (25)$$

by Gauss' theorem and the incompressibility condition. Thus, by applying Gauss' theorem to (7), one obtains

$$I = -\int (\partial u_i/\partial x_j)(\partial u_i/\partial x_k)(\partial u_j/\partial x_k)\,d^3x. \quad (26)$$

Now it is easy to verify by successive application of Gauss' theorem and the incompressibility condition that

$$\int (\partial u_i/\partial x_j)(\partial u_j/\partial x_k)(\partial u_k/\partial x_i)\,d^3x = 0. \quad (27)$$

As a consequence of (27), (26) is expressible as

$$I = -\frac{1}{6}\int (\operatorname{tr} S^3)\,d^3x, \quad (28)$$

where the symmetric traceless *rate-of-strain matrix* S has the elements

$$S_{ij} \equiv \partial u_i/\partial x_j + \partial u_j/\partial x_i. \quad (29)$$

For any real symmetric matrix M,

$$\operatorname{tr} M = 0 \Rightarrow |\operatorname{tr} M^3| \leqslant \frac{1}{(6)^{1/2}}(\operatorname{tr} M^2)^{3/2}, \quad (30)$$

as immediately shown by expressing the traces in terms of the real eigenvalues of M. Therefore (28) yields

$$I \leqslant \frac{1}{6(6)^{1/2}}\int (\operatorname{tr} S^2)^{3/2}\,d^3x, \quad (31)$$

while an upper bound on the trace of S^2 follows from (29) as

$$\operatorname{tr} S^2 = 2[(\partial u_i/\partial x_j)(\partial u_i/\partial x_j) + (\partial u_i/\partial x_j)(\partial u_j/\partial x_i)]$$
$$\leqslant 4(\partial u_i/\partial x_j)(\partial u_i/\partial x_j) \equiv 4|\nabla\mathbf{u}|^2. \quad (32)$$

Hence, (31) implies that

$$I < \left(\frac{2}{3}\right)^{3/2}\int |\nabla\mathbf{u}|^3\,d^3x, \quad (33)$$

with strict inequality holding because (26) vanishes [by virtue of (27)] for the case of equality in (32).

The lower bound on the maximum velocity gradient at time t, $|\nabla\mathbf{u}|_{\max} \equiv \max_{\mathbf{x}}|\nabla\mathbf{u}(\mathbf{x},t)|$, is obtained directly from (33), (4), (5), and (13) as

$$|\nabla\mathbf{u}|_{\max} \geqslant A_1^{-1}\int |\nabla\mathbf{u}|^3\,d^3x > (1.837)A_1^{-1}I$$
$$= (0.9186)[A_1^{-1}\dot{A}_1 + 2\nu(B+1)A^{-1}A_1]. \quad (34)$$

Finally, by using (3) to eliminate A_1 from (34) we have the result

$$|\nabla\mathbf{u}|_{\max} > (0.9186)[\dot{A}^{-1}\ddot{A} - (B+1)A^{-1}\dot{A}]. \quad (35)$$

In the case of freely decaying isotropic homogeneous turbulence, theory[9] and experiment give $A \propto t^{-n}$ for $t > t_0(>0)$ with $n(>1)$ and B quasiconstant with time; thus it follows from (35) that

$$|\nabla \mathbf{u}|_{\max} > (0.9186)(Bn-1)t^{-1}. \tag{36}$$

Derived here as a rigorous and general concomitant of the Navier–Stokes inertial-force nonlinearity, (36) is a remarkable bound on the decay of $|\nabla \mathbf{u}|_{\max}$ in isotropic homogeneous turbulence. This result is most interesting for the experimental values[9] $n = 3.3$, $B = 37.0$, which also give $\langle |\nabla \mathbf{u}|^2\rangle^{1/2} \propto t^{-2.15}$; for this type of very high Reynolds number turbulence, the dominant inertial force sustains a local $|\nabla \mathbf{u}|_{\max}$ which decays more slowly than the average velocity gradient $\langle |\nabla \mathbf{u}|^2\rangle^{1/2}$.

[1] J. Serrin in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1959), Vol. 8, Pt. 1, pp. 251–262.

[2] C. B. Millikan, Philos. Mag. **7**, 641 (1929).

[3] J. C. Slattery, Chem. Eng. Sci. **19**, 801 (1964).

[4] B. A. Finlayson, Phys. Fluids **15**, 963 (1972).

[5] G. Rosen, Phys. Fluids **21**, 695 (1978) and works cited therein.

[6] For example, P. M. Morse and H. Feshbach, *Methods of Thoretical Physics* (McGraw-Hill, New York, 1953), Vol. I, p. 313. In the case of (1) the adjoint-field variational principle is

$$\delta Q \equiv Q[\mathbf{u}+\delta\mathbf{u},\mathbf{v}+\delta\mathbf{v}] - Q[\mathbf{u},\mathbf{v}] = 0,$$

$$Q[\mathbf{u},\mathbf{v}] \equiv \int_{t'}^{t''} \int (\partial\mathbf{u}/\partial t + \mathbf{u}\cdot\nabla\mathbf{u} - \nu\nabla^2\mathbf{u})\cdot\mathbf{v}\, d^3x\, dt,$$

where $\nabla\cdot\mathbf{v} \equiv 0$ and $\mathbf{v} = 0$ for $t = t', t''$.

[7] For example, L. Hörmander, *Linear Partial Differential Operators* (Academic, New York, 1964), p. 2.

[8] More precisely, the minimum principle implies that $\mathbf{u}$ is a weak solution in the sense of A. A. Kiselev and O. A. Ladyženskaya [Izv. Akad. Nauk SSSR Ser. Mat. **21**, 655 (1957)]. It was shown by J. Serrin [in *Nonlinear Problems*, edited by R. E. Langer (U. Wisconsin P., Madison, WI, 1963), p.69] that a weak solution is in fact a classical solution to (1).

[9] G. Rosen, Phys. Rev. A **22**, 2180 (1980).

[10] G. Rosen, Phys. Fluids **13**, 2891 (1970). The proof of this inequality is based on the Green's function identity

$$\mathbf{u}(\mathbf{x},t) \equiv \int \left(\frac{\exp(-\mu|\mathbf{x}-\mathbf{y}|)}{4\pi|\mathbf{x}-\mathbf{y}|}\right)(\mu^2 - \nabla^2)\mathbf{u}(\mathbf{y},t)\, d^3y, \text{with } \mu = \mu(t) \text{ an}$$

arbitrary disposable positive function. Applying the Schwarz inequality to the latter identity, one obtains

$$|\mathbf{u}(\mathbf{x},t)|^2 \leqslant (8\pi\mu)^{-1}(\mu^4 A + 2\mu^2 A_1 + A_2)$$
$$\leqslant (8\pi\mu)^{-1}(\mu^2 A^{1/2} + A_2^{1/2})^2 \leqslant (2/3[3^{1/2}]\pi) A^{1/4} A_2^{3/4}$$

by setting $\mu = 3^{-1/2} A^{-1/4} A_2^{1/4}$. This is a strict inequality for $|\mathbf{u}|^2_{\max}$, because the intermediate cases of equality are mutually exclusive.

[11] A. Dold and B. Eckmann, editors., *Turbulence and the Navier-Stokes Equation*, Lecture Notes in Mathematics No. 565 (Springer, New York, 1976).

Distorted black holes

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All exact solutions of Einstein's equation that represent static, axisymmetric black holes distorted by an external matter distribution are obtained. Their structure—local and global—is examined. The Hawking temperature is derived and laws of thermodynamics given for both the total system of black hole and external matter and the black hole considered as a single system. The evolution, induced by Hawking radiation, of distorted black holes is discussed.

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1. INTRODUCTION

By far the largest part of our insight into the structure of black holes has come from the study of two families of exact solutions—the Schwarzschild and Kerr. For these examples, a great deal is now understood about their local and global classical geometries, their roles as backgrounds for quantum fields, and their behavior as thermodynamic systems.[1] To what extent are the properties of these examples a reliable guide to those of more general black holes? Might there be new, unexpected effects, either classical or quantum, associated with holes that, for one reason or another, do not happen to appear in these examples? Complete answers to such questions would presumably involve finding the general, dynamical exact solution for a black hole—something that seems far out of reach. But hints and partial answers can be obtained, along at least two lines.

One is to study approximate solutions. A great deal is known, for example, about the behavior of first-order perturbations off the Schwarzschild and Kerr solutions.[2] Further, computer calculations have been carried out for the dynamical evolution of holes under various situations.[3] The great advantage of these approaches is that one often retains the flexibility to tailor the approximate solution to a realistic astrophysical situation, e.g., the incidence of gravitational waves on a hole, or the coalescence of two black holes.

A second line is to increase our supply of exact solutions representing black holes. It might be expected, as has happened before, that qualitatively different effects would show up most readily in such exact solutions. The problem is that restrictive, simplifying conditions must be imposed to even begin, and there tends to be little flexibility in the choice of these conditions. Indeed, it is not easy offhand to think of any good candidates, for the only isolated static or stationary black holes are Schwarzschild or Kerr,[4] while dynamical solutions suggest equations not readily solved.

There is, however, one class of solutions for black holes that is amenable to exact treatment: Retain the time-independent character but drop the condition "isolated." That is, consider static or stationary holes in the presence of some external distribution of matter. Such solutions should approximate those for dynamical holes which relax on a time scale much shorter than that of the external matter. Further simplification results from considering only holes that are static (as opposed to stationary), and also axisymmetric. Now the external metric near the hole must be a Weyl solution, and all these are essentially known.[5]

General classes of Weyl solutions representing black holes of spherical horizon-topology distorted by external matter have been discussed by Israel and Khan,[6] Mysak and Szekeres,[7] and Israel.[8] An example in which the horizon has toroidal topology has been constructed by Peters.[9] However, all holes in this class have apparently not yet been found and classified. In Sec. 2, we find all static, axisymmetric local black holes. The problem is not so much to determine the metric—for it is Weyl—but rather to determine which Weyl solutions are and which are not black holes. It turns out that spherical and toroidal are the only possibilities for the topology of horizon cross sections. The spherical class consists essentially of the solutions given in Refs. 6–8. The Peters example is but one of the many possibilities in the toroidal class.

In Sec. 3, we discuss various classical properties of the holes. Simple expressions are obtained for their mass, horizon-area, and surface gravity. The spherical holes turn out to have virtually the same qualitative features—as regards their singular behavior as well as the location and topology of external regions, horizons, crossing points, and internal regions—as the Schwarzschild holes. The global properties of the toroidal holes are also explored.

The solutions with distorted black holes are natural examples for explicit study of the laws of black-hole mechanics and thermodynamics—the laws that describe how such systems change under variations in their external environment. Israel has studied some properties of these solutions in this connection.[8] In Sec. 4, we discuss the mechanics and thermodynamics of the Weyl black holes. While of course the usual, general laws, appropriate to the system of hole plus external matter, are here applicable, we find further that laws can be formulated for Weyl black holes considered as single systems, acted upon by the tidal gravitational forces of the external matter.

In Sec. 5, we treat the evolution, which results from the Hawking radiation, of the distorted Weyl black holes. A peculiarity of the Weyl construction allows a simple description of this evolution in terms of a background potential.

Finally, in Sec. 6 we show that the results of the previous two sections—the local laws of thermodynamics and the description of the evolution—can for the most part be generalized to include all static distorted holes.

2. THE WEYL BLACK HOLES

We first recall the Weyl construction.[5] Since we wish to retain the possibility of holes involving nontrivial topology, we state this construction in global form.

Let S be a connected orientable, three-dimensional manifold, h_{ab} a flat, positive-definite metric on S, and φ^a a Killing field for (S,h_{ab}) that is "rotational" in the sense that, with $r^2 = \varphi^a\varphi_a$, we have $D^a r\, D_a r = 1$. Ordinary Euclidean space with the usual rotational Killing field is of course one example, but, because we have imposed no global conditions, there are numerous others. Writing out, in a local region of the flat space, all Killing fields, one sees that our normalization condition on r implies that φ^a is surface orthogonal, and, conversely, that any nonconstant surface-orthogonal Killing field φ^a can be rescaled by a constant to achieve $D^a r\, D_a r = 1$. By the *axis* we mean the set of points of S, if any, at which $r = 0$. Our normalization of r also implies that, near any axis point, the orbits of φ^a are closed curves of period 2π.

Now let U be any smooth function on S satisfying the equations

$$D^aD_a U = 0, \quad \varphi^a D_a U = 0, \tag{2.1}$$

where D_a is the derivative operator associated with h_{ab}. Let V be any smooth function that satisfies

$$D_a V = \left[\delta_a{}^m D^n(r^2) - \tfrac{1}{2}h^{mn}D_a(r^2)\right] D_m U D_n U, \tag{2.2}$$

and that vanishes on the axis. Note that the right-hand side of (2.2) is smooth, and, by virtue of (2.1), has vanishing curl. So, a solution V of (2.2) always exists locally—but of course not in general globally. By adding a constant to V, one can always achieve its vanishing at one axis point. Then, since the right-hand side of (2.2) vanishes identically at all axis points, this V will vanish on the entire portion of the axis connected to that point. However, when the axis consists of several pieces, the resulting V will not in general then vanish at all axis points. So, U must be chosen such that it does. Finally, note that, by (2.2), V is also axisymmetric: $\varphi^a D_a V = 0$.

Now let $M = S \times \mathbb{R}$, let t^a denote the natural vector field on M in the $\mathbb{R}$ direction, and regard tensor fields on S as fields on M. Then the Weyl metric

$$g^{ab} = e^{2U-2V}h^{ab} + r^{-2}e^{2U}(1 - e^{-2V})\varphi^a\varphi^b - e^{-2U}t^a t^b \tag{2.3}$$

on M is a solution of Einstein's equation with vanishing stress energy. This space-time has commuting, orthogonal, surface-orthogonal Killing fields t^a (complete and everywhere timelike, with squared norm $-e^{2U}$) and φ^a (with squared norm r^2e^{-2U}).

It is shown in Appendix A that, aside from certain anomalous cases, every static, axisymmetric solution can be written in Weyl form, (2.3), and that this characterization is essentially unique.

The most famous Weyl solution is the external Schwarzschild solution.[10] Let (S,h_{ab}) be Euclidean space, in ordinary cylindrical coordinates r,z,φ, but with a segment H of the axis, of length $2m$ (m some positive number), centered at the origin removed from S. Let φ^a be the rotational Killing field in the "φ direction." Set

$$U_S = \tfrac{1}{2}\ln[r^2(m - z + ((m-z)^2 + r^2)^{1/2})^{-1} \times (m + z + ((m+z)^2 + r^2)^{1/2})^{-1}], \tag{2.4}$$

the potential of a line mass, of unit density, located on H. This U_S satisfies (2.1). Let V_S be that solution of (2.2) which vanishes on the axis of S (H excluded). Then (2.3) for these choices is precisely the external Schwarzschild solution of mass m. The Schwarzschild horizon is "at H." The present coordinates r and z are related to the standard Schwarzschild coordinates, r_S and θ_S, by the formulas

$$r^2 = r_S(r_S - 2m)\sin^2\theta_S,\ z = (r_S - m)\cos\theta_S. \tag{2.5}$$

The external Schwarzschild solution of course represents a static, axisymmetric (indeed, spherically symmetric) isolated black hole. We now wish to identify those Weyl solutions which represent nonisolated holes, i.e., those in the presence of some static, axisymmetric external gravitational field. To this end, we say that a four-dimensional Weyl solution (2.3) is a *local black hole* if it has an extension to a true static black hole such that the original Weyl solution forms a neighborhood of the horizon in the external region. In more detail, we require of the extension that it be asymptotically flat at null infinity, retain t^a as a complete Killing field that becomes a unit time-translation asymptotically, and have a future horizon (i.e., a null surface that separates points from which there is a future-directed timelike curve to null infinity from those from which there is not) that is connected and nonsingular (i.e., of the form $C \times \mathbb{R}$ with the $\mathbb{R}$'s the null generators and the C's compact, connected cross sections). The reasons for this definition are the following. First, since the Weyl solutions come with vanishing stress energy, they will not include explicitly the matter distribution responsible for the "external gravitational field." We accommodate this fact by letting our Weyl solution represent only a neighborhood of the hole itself, with this external matter, implicitly, in the extension. Note that, out of convenience, we impose no energy condition on the external matter. Next, recall that the horizon of a static black hole is the set of points at which the static Killing field becomes null.[11] Hence, since t^a is strictly timelike in any Weyl solution, this solution cannot include the actual horizon points. For this reason, we demand only that the Weyl solution be an external neighborhood of the horizon. Note that essentially no conditions have been imposed above on the topology of either the horizon or the space-time in its neighborhood.

Fix a local black hole. Then, since the norm of t^a, $-e^{2U}$, approaches zero on the horizon, while the norm of φ^a, r^2e^{-2U}, must remain bounded, their product, r^2, must vanish on the horizon. That is, the horizon must appear "as $r\to 0$" in the Weyl solution. It is shown in Appendix B that the topology of a cross section C of the horizon must be that of either a torus or a sphere. Intuitively, φ^a either vanishes nowhere on C (resulting in a torus), or has a zero-point (resulting, on working outward from this point, in a sphere). There is further analyzed, in Appendix B, the detailed behavior of h_{ab} and U as $r\to 0$ which is necessary in order that extension through a horizon actually be possible. With the convention that two holes are regarded as "the same" if they coincide in some neighborhood of the horizon, there results the following list of all local black holes.

The spherical holes have been obtained in Refs. 6–8. Let H be the line segment of length $2m$ centered at the origin in Euclidean 3-space as in the Schwarzschild example, let $\bar{S}$ be any small open neighborhood of H, and set $S = \bar{S} - H$. Set $U = U_S + \hat{U}$, where U_S is given by (2.4) and $\hat{U}$ is any smooth solution of (2.1) on $\bar{S}$, i.e., including H, such that $\hat{U}$ assumes the same values,[12] u, on the two ends of the segment H. These choices, we claim, always yield a local black hole.

We first show the existence of an extension through a horizon. Set $V = V_S + \hat{V}$, where V_S is the Schwarzschild function, and substitute into (2.2):

$$D_a \hat{V} = [\delta_a{}^{(m} D^{n)}(r^2) - \tfrac{1}{2} h^{mn} D_a(r^2)] \times (2 D_m U_S D_n \hat{U} + D_m \hat{U} D_n \hat{U}). \tag{2.6}$$

Consider now the metric

$$g_S^{ab} = e^{2U_S - 2V_S} h^{ab} + r^{-2} e^{2U_S}(1 - e^{2V_S}) \varphi^a \varphi^b - e^{-2U_S} e^{-4u} t^a t^b. \tag{2.7}$$

This will be recognized, from (2.3), as the exterior Schwarzschild metric of mass m, with "the time rescaled by a constant." Rewrite our Weyl metric, (2.3), in the form

$$g^{ab} = e^{2\hat{U} - 2\hat{V}} g_S^{ab} + r^{-2} e^{2U_S} e^{2\hat{U}} (1 - e^{-2\hat{V}}) \varphi^a \varphi^b - e^{-2U_S} e^{-2\hat{U}} (1 - e^{4\hat{U} - 4u - 2\hat{V}}) t^a t^b. \tag{2.8}$$

The plan is to find an extension of the metric g^{ab} on M by extending each of the tensor fields on the right in (2.8). First, take the usual full Kruskal extension to manifold $\bar{M}$, of the Schwarzschild metric $g_S{}^{ab}$, and extend each of $\varphi^a \varphi^b$ and $t^a t^b$ from M to $\bar{M}$ by retaining its character as the square of a Killing field of $g_S{}^{ab}$. There remains only to extend to $\bar{M}$ the coefficients of $g_S{}^{ab}, \varphi^a \varphi^b$, and $t^a t^b$ in (2.8). To extend $\hat{U}$, first note that, as an axisymmetric solution of Laplace's equation in a neighborhood of H, $\hat{U}$ is an analytic function of the variables r^2 and z, for r^2 sufficiently small and positive and z sufficiently close to the interval $[-m, m]$. Analytically extend $\hat{U}$ as a function of these variables, and substitute from (2.5).[13] Next, extend $\hat{V}$ to $\bar{M}$ by (2.6), verifying, from smoothness of $\hat{U}$, that the right side is smooth. Finally, recombine these extensions of $g_S{}^{ab}, \varphi^a \varphi^b, t^a t^b, \hat{U}$, and $\hat{V}$ to M, according to (2.8), to obtain our extension of the Weyl metric g_{ab}. There remains only to check smoothness of the coefficients of $\varphi^a \varphi^b$ and $t^a t^b$ on the right in (2.8). For the first, note from (2.6) that $\hat{V}$, and so the smooth combination $e^{2\hat{U}}(1 - e^{-2\hat{V}})$, is axisymmetric and vanishes on the axis. But $r^2 e^{2U_S}$ is the squared norm of the rotational Killing field φ^a in $g_S{}^{ab}$, and so their quotient, the coefficient of $\varphi^a \varphi^b$ in (2.8), is smooth. Similarly, to see that the coefficient of $t^a t^b$ is smooth, first note that the smooth combination $e^{-2\hat{U}}(1 - e^{4\hat{U} - 4u - 2\hat{V}})$ vanishes on the horizon, as one checks by integrating (2.6) along a straight line parallel to and near H, beginning at one end. [It was to achieve this vanishing that we inserted the "e^{-4u}" into the last term of (2.7).] But e^{2U_S}, the squared norm of t^a in $g_S{}^{ab}$, also vanishes on the horizon, with nonzero gradient there, and so their quotient is smooth.[14]

We next show the existence of an extension that achieves asymptotic flatness. This is easy. Extend S as a manifold, h_{ab} as a Riemannian metric, φ^a as a vector field, and U and V as scalar fields—not necessarily retaining flatness of h_{ab}, the Killing character of φ^a, or Eqs. (2.1) and (2.2) on U and V—such that (S, h_{ab}) is asymptotically Euclidean, φ^a is asymptotically a rotational Killing field, and U and V are asymptotically zero. Now substitute into (2.3) to obtain the desired extension. Note that the failure to satisfy (2.1) and (2.2), in particular, will result in matter in the external region.

For the second class of local black holes, the toroidal, the background Schwarzschild metric above is replaced by certain flat Weyl solutions. Consider again Euclidean 3-space, in cylindrical coordinates (r, z, φ) and with φ^a the rotational Killing field, but only that portion with $-m \leqslant z \leqslant m$, where m is some positive number. Now identify points labeled $(r, -m, \varphi)$ with those labeled $(r, m, \varphi + \alpha)$, where α is a constant. That is, we make the z coordinate cyclic, with period $2m$, at the same time introducing a φ twist through angle α. Denote the axis (a circle of circumference $2m$) by H, and again let $\bar{S}$ be a small open neighborhood of H and set $S = \bar{S} - H$. Thus, S is a three-dimensional manifold with positive-definite flat metric h_{ab} and rotational Killing field φ^a. Next, let $U_T = \ln(r/2m)$, a solution of (2.1) on S, and $V_T = \ln(r/m)$, a solution of (2.2). (For later convenience, the constants have been so chosen as to give agreement with the behavior of U_S and V_S near the center of H in the Schwarzschild case.) Then (2.3) yields a corresponding Weyl solution, which, in the present coordinates, takes the form

$$ds^2 = 4dr^2 + 4dz^2 + 4m^2 d\varphi^2 - (r^2/4m^2) dt^2. \tag{2.9}$$

This will be recognized as a flat space-time, consisting of the product of a twisted flat torus (labeled by z and φ, with the identifications above) and a region of two-dimensional Minkowski space (labeled by r and t), namely that region in which the boost Killing field t^a is future-directed timelike.

These flat Weyl solutions are clearly local black holes. The extension through a horizon is that obtained by extending the region of Minkowski 2-space above through the two null lines "$r = 0$." An extension to achieve asymptotic flatness is obtained by the same argument as in the spherical case. In fact, one can achieve such an extension with, in an appropriate sense, a nonsingular external region. First choose S to have as outer boundary a torus, then choose an asymptotic region with inner boundary a 2-sphere, and finally join these two using the fact that there exists a compact 3-manifold with boundary consisting of the disjoint union of a torus and a sphere (namely, the result of removing an open solid torus from a 3-ball). All such extensions will have negative mass in the external region, as a theorem of Hawking shows.[15]

We now obtain the distorted versions of these toroidal holes, by an argument similar to that above for the spherical holes. Set $U = U_T + \hat{U}$, where $\hat{U}$ is any smooth solution of (2.1) on $\bar{S}$, i.e., including H. There results from (2.3), we claim, a local black hole. Set $V = V_T + \hat{V}$, and substitute into (2.2):

$$D_a \hat{V} = 2 D_a \hat{U} + [\delta_a^m D^n(r^2) - \tfrac{1}{2} h^{mn} D_a(r^2)] D_m \hat{U} D_n \hat{U}. \tag{2.10}$$

It follows that $\hat{U} - \frac{1}{2}\hat{V} = u$ approaches a constant on H, and from this that a solution $\hat{V}$ of (2.10) always exists globally in S. Now set

$$g_T^{ab} = e^{2U_T - 2V_T} h^{ab} + r^{-2} e^{2U_T} (1 - e^{-2V_T}) \varphi^a \varphi^b - e^{-2U_T} e^{-4u} t^a t^b, \tag{2.11}$$

i.e., (2.9) with time rescaled by a constant, and rewrite our Weyl metric, (2.3), in the form

$$g^{ab} = e^{2\hat{U} - 2\hat{V}} g_T^{ab} + r^{-2} e^{2U_T} e^{2\hat{U}} (1 - e^{-2\hat{V}}) \varphi^a \varphi^b - e^{-2U_T} e^{-2\hat{U}} (1 - e^{4\hat{U} - 4u - 2\hat{V}}) t^a t^b. \tag{2.12}$$

The extension through a horizon is obtained exactly as in the spherical case. First extend the 4-manifold M and $g_T{}^{ab}$ as for the flat toridal holes above; then $\varphi^a \varphi^b$ and $t^a t^b$ retaining their character as squares of Killing fields; then $\hat{U}$ using its analyticity in z and r^2; and finally $\hat{V}$ using (2.10). Then recombine according to (2.12). The check of smoothness is much easier in this case. An extension to achieve asymptotic flatness is the same as that for the flat toridal holes. A particular hole in this class has been studied by Peters.[9,16]

Thus, we obtain two broad classes, spherical and toroidal, which, by Appendix B, include all Weyl local black holes.

3. STRUCTURE OF THE BLACK HOLES

It follows from (2.8) and (2.12) that our extended solutions for distorted holes have all the qualitative features of their undistorted versions—the extended Schwarzschild solution for the spherical holes and the flat space-times, as extended, for the toroidal. In particular, the distorted holes all have two horizons, each a null surface topologically $S^2 \times \mathbb{R}$ for the spherical or $S^1 \times S^1 \times \mathbb{R}$ for the toroidal. The generators of these horizons are given by the static Killing field. The two horizons meet on a topological 2-sphere (2-torus), on which the static Killing field vanishes. From the external region, one can cross one of the horizons in the future timelike direction, or the other in the past, and in either case reach an internal region, in which the static Killing field is spacelike. These two internal regions"touch" on the 2-sphere (2-torus) at which the horizons intersect. From the viewpoint of an external observer, there is both a black hole and a white hole. Going "through the wormhole," one crosses a second horizon and reaches a second external region. Its geometry can be identical to that of the original external region, but the static Killing field is there past-directed. The two external regions "touch" on the 2-sphere (2-torus) at which the horizons intersect. No timelike curve can pass from one external region to the other. Of course there are, globally, many other extensions of the external metrics of the distorted holes, just as there are for the external Schwarzschild space-time.

We also see from the constructions leading from (2.8) and (2.12) that our extended distorted holes have vanishing sources in the internal regions. Further, the distortion introduces no "new singular behavior" inside the horizon, in the sense that (2.8) and (2.12) are smooth wherever $g_S{}^{ab}$ and $g_T{}^{ab}$ are, respectively. Thus, in the spherical case, we expect that each internal region terminates in singular behavior, one to the past and one to the future. For the toroidal holes, the undistorted backgrounds are nonsingular in the internal regions. Thus, it is possible that for all or a large class of choices of the potential $\hat{U}$ these holes are geodesically complete. The toroidal holes have no trapped surfaces just inside the horizon. All the distorted holes require external matter. Whereas for toroidal holes this matter cannot satisfy an energy conditon everywhere,[15] it seems likely that for certain spherical holes—those with u sufficiently negative—it can.

Since the horizons are null and are generated by a Killing field, all cross sections of the horizons (topologically, spheres or tori) have the same geometry. For the undistorted holes these are, of course, metric 2-spheres or certain twisted flat tori. For the distorted holes, the geometry can be read all directly from Eq. (2.8) or (2.12).

A local distorted black hole in the spherical case is uniquely characterized by specifying the length, $2m$, of the segment H on the axis in Euclidean space, together with an axisymmetric solution, $\hat{U}$, of Laplace's equation, defined in a neighborhood of H and having the same value u at the two ends of H. Since the horizon occurs "at H," and since there $\hat{V} = 2\hat{U} - 2u$, the geometry of the horizon is uniquely determined by $\hat{U}$ evaluated on H, i.e., by the one function of one variable, $\hat{U}(z)$, defined for $-m \leqslant z \leqslant m$. Evaluating the horizon geometry from (2.8), we obtain the metric

$$ds^2 = 4m^2 e^{-2u} [e^{2\hat{U} - 2u} d\theta^2 + e^{2u - 2\hat{U}} \sin^2 \theta \, d\varphi^2], \tag{3.1}$$

where $\hat{U}$ is made a function of θ by substituting $z = m \cos \theta$. This is an axisymmetric—but not in general spherically symmetric—metric on a topological 2-sphere. All analytic (since $\hat{U}$ necessarily is) axisymmetric horizon geometries are possible. As an intuitive example, suppose that $\hat{U}$ were larger near the ends of H (z near $+m$ and $-m$) than near the middle (z near zero). Then (3.1) would represent a 2-sphere "squashed inward on its poles."

Similarly, the toroidal holes are characterized by value of m, the "twist parameter" α, a certain axisymmetric solution $\hat{U}$ of Laplace's equation, and the constant value u of $\hat{U} - \frac{1}{2}\hat{V}$ on approaching the horizon. As above, only $\hat{U}$ on the axis, i.e., only the function $\hat{U}(z)$, defined for $-m \leqslant z \leqslant m$ and periodic, enters the horizon geometry. From (2.12), we obtain the metric

$$ds^2 = 4e^{-2u} [e^{2\hat{U} - 2u} dz^2 + m^2 e^{2u - 2\hat{U}} d\varphi^2], \tag{3.2}$$

where φ has period 2π, z ranges from $-m$ to m, and $(-m, \varphi)$ and $(m, \varphi + \alpha)$ are identified. The geometry is that of a twisted torus with Killing field, and, again, all analytic ones are possible.

In the spherical case, we may interpret physically the distortion of the geometry of the horizon, as follows. Fix a distorted hole, characterized by $2m$ and $\hat{U}$. Consider now the Weyl solution defined by $U = \hat{U}$, a solution that of course is smooth up to and including H. We may think of this solution as representing "the background gravitational field caused by the external masses alone, with no hole present." Then our distorted hole, the Weyl solution defined by $U = U_S + \hat{U}$, would represent "the combination of a Schwarzschild hole and this background gravitational field." It seems to be difficult to make these remarks precise, because of all the usual problems of comparing two different metrics. But this interpretation is at least suggested by the fact that U_S, the Schwarzschild potential given by (2.4), approaches zero far from H. Thus, the two Weyl solutions (the distorted hole, given by $U = U_S + \hat{U}$, and what we wish to call the background field, given by $U = \hat{U}$) are in some sense "nearly equal far from the hole." But this is what we would expect physically: A black hole, placed in a background gravitational field, should have a small effect on the distant external mass distribution responsible for that field. Presumably, this interpretation is most appropriate for small holes and distant matter.

In any case, let us for a moment accept this interpretation. Then we may think of a black hole as an elastic body, subject to Hooke's law. The stress is the Weyl tensor of the background metric, evaluated on H; the strain is the horizon geometry (3.1) (or, more precisely, its deviation from spherical). It is not difficult to write out explicitly the stress–strain relation. But this formula is not very illuminating, for both the stress and strain have an infinite number of degrees of freedom. One can, however, see intuitively that the "elastic constant" has the correct sign. Consider the case in which $\hat{U}$ is larger near the ends of the segment H than near its center. Then a free test particle, released at rest near one end of H in the background geometry, will tend to fall inward toward the center of H. That is, a test physical object, placed near H in the background field, will tend to be "pushed inward from the ends of H." But this agrees with our interpretation of the horizon geometry, (3.1), in this case.

It is also possible to interpret physically the condition in the spherical case that $\hat{U}$ assume the same value at the two ends of the segment H. Consider a test particle, released initially at rest (i.e., with its four-velocity parallel to the static Killing field t^a) in the background field. Then this particle will remain at rest if and only if the gradient of $\hat{U}$ vanishes at the location of the particle. Otherwise, it will feel a force from the gravitational field, and move off. So, if a black hole—an extended object—were to be placed in this field, we would expect some similar condition—the vanishing of some average of the gradient of $\hat{U}$—in order that the hole experience no net force, and so remain at rest. The difference between the values of $\hat{U}$ at the two ends of H is the appropriate average.

Is there an analogous separation of the solutions for distorted toroidal holes into one solution representing the undistorted hole and another representing the background gravitational field into which it has been placed? There is, but the interpretation is somewhat less clearcut in this case. Given a distorted hole, defined by the parameters $2m$ and α and the Laplace solution $U = U_T + \hat{U}$, we may certainly consider the two Weyl solutions given by $U = U_T$, the "undistorted hole," and by $U = \hat{U}$, the "background gravitational field." But note, first, that the parameters m and α for the distorted hole enter the Weyl solutions for both the undistorted hole and the background field. Thus, we are forced to regard the background field, which fixes both m and α, as an arena in which can be placed only certain undistorted holes, namely those with the same values of m and α. A second complication involves the interpretation of the parameter u as an "effective potential" of the background field at the location at which the hole is to be placed. Such an interpretation is at least reasonable in the spherical case, for there u is determined from $\hat{U}$, as its values at the ends of H. But, in the toroidal case, u arises only at the point, in writing down the full distorted solution, at which we must choose the constant in $\hat{V}$. [This freedom disappears in the spherical case, because there we must require vanishing of $\hat{V}$ on that part of the axis away from the horizon.] In short, the physical meaning of u in the toroidal case is by no means clear. A final difficulty is that the interpretation of the solution with $U = U_T$ as the "undistorted hole" is weakened by the fact that these local black holes, if fully extended to achieve asymptotic flatness, must necessarily contain external matter. This circumstance constrasts with the spherical case, in which the undistorted holes are Schwarzschild solutions, which require no such external matter.

Our parameters have been so chosen that the masses of all the spherical and toroidal holes—defined using the Komar integral with the static Killing field t^a of (2.3)—are just m. In particular, even the flat, undistorted toroidal holes have nonzero mass! The area of the horizon is obtained by integrating (3.1) for spherical, or (3.2) for toroidal:

$$A = 16\pi m^2 e^{-2u}. \tag{3.3}$$

Thus, the Schwarzschild mass–area relationship is in general violated for the distorted holes. But this is exactly what one expects physically. The mass defined by $(A/16\pi)^{1/2}$ is analogous to the rest mass of a particle, $(-p^a p_a)^{1/2}$, where p^a is the four-momentum. The Komar mass m is analogous to $-p_a t^a$. For a particle at rest (p^a parallel to t^a), these two differ by a redshift factor, essentially the norm of t^a. But this redshift factor appears in (3.3), as "e^{-2u}." Note that the hole looks to the ends of the segment H to decide what redshift factor to assume.

For both the spherical and toroidal holes, the surface gravity,

$$\kappa^2 = \lim \tfrac{1}{2}(\nabla_a t_b)(\nabla^a t^b) = \lim e^{4U-2V} h^{ab} D_a U D_b U, \tag{3.4}$$

where the limit is at the horizon, is given by

$$\kappa = (4m)^{-1} e^{2u}. \tag{3.5}$$

Note that $\kappa A/m = 4\pi$ for all holes, independent of topology and distortion.

4. MECHANICS AND THERMODYNAMICS OF DISTORTED BLACK HOLES

The work of Bekenstein[17] and Hawking[18] has shown, and that of many others confirmed, that the mechanical laws governing classical systems containing black holes can be placed in analogy with those of thermodynamics. Further, the resulting correspondence between mechanical black-hole variables (horizon area, surface gravity, etc.) and thermodynamic variables (entropy, temperature, etc.) has independent physical meaning when quantum mechanics is taken into account. This correspondence has been made explicit for a number of examples, including the Kerr black holes. In this section, we first review this work as it applies to the systems of black hole plus distorting matter considered in the previous sections. In the process we obtain explicit expressions for the temperature and entropy of the distorted black holes. Next, using the natural decomposition of the Weyl potential U into pieces assignable to the black hole and distorting matter, we go slightly further. We consider the black hole as a single system acted upon by the gravitational forces of the external matter, and find that its laws continue to have a simple correspondence with those of thermodynamics.

We begin our discussion of the thermodynamics of distorted black holes by deriving the Hawking temperature.[19] Consider quantum particles in the background space-time of a distorted black hole. One expects there to be particle states inside the horizon that have negative energy when viewed from infinity. The ability of the system to occupy such states should then give rise, by pair creation, to Hawking radiation of particles at infinity. While the determination of all the details of this radiation is in general difficult, there is a simple argument that yields certain general features. Imagine placing the black hole in a large, suitably confining box, together with radiation at some temperature. Is there some temperature for this radiation such that the resulting system will be in thermal equilibrium? If so, then one expects that the radiation from the free hole will be thermal with precisely this temperature. As Gibbons and Perry[20] have shown, the existence and value of such an equilibrium temperature can be determined directly from the static space-time geometry. They argue that it is a *general* property of thermal equilibrium that the thermal Green's function of the quantum fields, with Killing time t replaced by it, become periodic in this "complex Killing time," with period the inverse of the equilibrium temperature. Conversely, the existence of a periodicity in complex Killing time should allow the construction of a thermal Green's function.

Thus, the Gibbons–Perry prescription for determining the existence and value for the temperature of thermal equilibrium for a static black hole is the following. First, write the metric in the external region in the form

$$g_{ab} = -e^{-2U}t_a t_b + \gamma_{ab}, \tag{4.1}$$

where $\gamma_{ab}t^b = 0$ and $t^a t_a = -e^{2U}$. Next, introduce Killing time t—such that t^a and $\nabla_a t$ are parallel and $t^a\nabla_a t = 1$. Then, on that part of the space–time manifold external to the horizon, introduce the positive-definite metric that results from reversing the sign of the first term on the right in (4.1). Now consider any positive number p (a candidate for the period), and identify, in this external space, all points lying on the same t^a-orbit and having t-values that differ by p. Find those p's, if any, such that the positive-definite metric on this identified manifold can be extended to include an axis of t^a (a "bolt" in the terminology of Gibbons and Hawking)[21] at $e^{2U} = 0$, i.e., where the horizon was. If such a period p exists (easily shown to be unique, in the presence of a horizon), then $1/p$ is the equilibrium temperature. It is not difficult to show that, if the space–time contains a compact horizon-crossing 2-surface, on which t^a vanishes, then there necessarily exists such a p, for this surface becomes the axis of t^a.

A consequence of the Gibbons–Perry prescription is a simple formula for the equilibrium—and hence radiation—temperature of a static black hole in terms of the surface gravity[22]:

$$T = \kappa/2\pi. \tag{4.2}$$

This is immediate from the first equality in (3.4).

Some remarks are in order concerning the physical meaning of this temperature. At infinity, the Green's function will approach the Green's function for flat space-time appropriate to a system in thermal equilibrium. With the Killing field t^a normalized to unity at infinity (a normalization we will henceforth assume), the temperature T given by (4.2) will be that measured by an ordinary thermometer at rest at infinity. This T will not, therefore, be the temperature measured by a static thermometer elsewhere in the space-time.[23] In the familiar way, a constituent of the gas moving freely through the space–time will preserve $p_a t^a$, where p_a is its 4-momentum. In equilibrium, this conserved energy must be the same everywhere in the gas. A static thermometer, however, measures energy relative to a *unit* vector parallel to t^a. Thus, the locally measured temperature differs from T by a redshift factor[24]:

$$T_{\text{loc}} = Te^{-U}. \tag{4.3}$$

All the distorted spherical and toroidal holes constructed earlier have a crossing surface, and so a Hawking temperature. From (3.5) and (4.2), this temperature is

$$T = (8\pi m)^{-1}e^{2u}. \tag{4.4}$$

In the spherical case with no distorting matter, and so with $u = 0$, (4.4) reduces, of course, to the Schwarzschild value. We claim that the effect of reasonable distorting matter in the spherical case is to lower the temperature from its Schwarzschild value. Indeed, in the presence of sources Einstein's equation projected along t^a reads

$$D^a D_a \hat{U} = 8\pi e^{2(\hat{U} - 2\hat{V})}(T_{ab} - \tfrac{1}{2}Tg_{ab})\, t^a t^b. \tag{4.5}$$

Under the strong energy condition, the right side is nonnegative, and therefore $\hat{U}$, and so u, is nonpositive. By (3.3), therefore, the effect of such distorting matter is to lower the temperature for fixed A (and also for fixed m)—the same direction as the effect of rotation. The effect of either spinning up or distorting an initially Schwarzschild black hole is always to lower its temperature. In the toroidal case, by constrast, while we still have (4.5), no conclusion as to the direction of temperature change from distortion is possible, not least because we cannot then impose the strong energy condition.

The laws of mechanics for an axisymmetric system consisting of black hole plus distorting matter have been given by Bardeen, Carter, and Hawking.[25] The zeroth law states that the surface gravity is constant over the horizon.[26] The first law states that, between two nearby equilibrium configurations,

$$\delta M = (\kappa/8\pi)\,\delta A + \delta Q, \tag{4.6}$$

where δM is the change in the total mass, δA is the change in horizon area, and δQ is a certain expression involving the change in the stress-energy of the external matter, interpretable as the change in its heat content as measured from infinity. The second law states that,classically, the area of the horizon is nondecreasing. With the temperature given by (4.2), the first law becomes identical with the first law of thermodynamics, provided the black hole is assigned an entropy equal to one quarter its area. The generalized second law can then for formulated in the usual way that the entropy of the black hole plus that of the external matter is nondecreasing.

The general laws above concern the total system, consisting of the black hole together with its distorting matter. They, of course, apply in particular to the spherical and toroidal holes of the previous sections. But for these we can write down further laws for the black hole regarded as a single system acted upon by external gravitational forces. The zeroth and second laws, being already local to the hole, remain unchanged. But various forms of the first law are available, depending on how the mass of the hole is characterized.

For example, using the Komar mass m, the mass of the hole alone as measured at infinity, one has from (3.3) and the identification of the thermodynamic variables

$$\delta m = T\delta S + m\delta u. \tag{4.7}$$

This is a version of the first law of thermodynamics, with the term $m\delta u =$ (mass of hole) $\times$ (change in external potential) interpreted as the work done on the hole by the variation in the external matter. This interpretation is confirmed by the observation that, for slow changes in which neither matter nor gravitational waves cross the horizon,[27] $\delta A = 0$, and so, by (4.7), $m\delta u$ is indeed the change in the mass m.

There is also a version of the first law appropriate to observers who, living near the hole, have no access to infinity. These observers cannot determine the Komar mass m, for they do not know how to scale the static Killing field t^a to make it unit at infinity. That is, these observers could determine the Weyl potential U only up to an arbitrary additive constant. At least in the spherical cases, they might resolve this ambiguity by computing U_S, the "potential due to the hole," and demanding that the difference, $U - U_S = \hat{U}$, vanish at the ends of the segment H. In this way, these observers would rescale the static Killing field by a redshift factor, and so would obtain for their mass of the hole

$$m_{\text{int}} = me^{-u}. \tag{4.8}$$

Then, from (3.3),

$$A = 16\pi m_{\text{int}}^{2}, \tag{4.9}$$

as we would expect for observers having access only to the hole. Similarly, these observers would measure locally a temperature, (4.3), for the radiation, i.e., a temperature that approaches infinity at the hole. They would attribute this effect to the local redshift caused be the hole, and so would correct it to an "ambient background temperature" using the redshift factor for the hole, e^{U_S}. Thus, their version of the temperature would be

$$T_{\text{int}} = Te^{-u} = (8\pi m_{\text{int}})^{-1}, \tag{4.10}$$

From (4.9) and (4.10), we obtain a local version of the first law

$$\delta m_{\text{int}} = T_{\text{int}}\delta S. \tag{4.11}$$

There is no work term in this version because these observers effectively ignore the overall potential due to the external matter. In the toroidal case, the definitions (4.8) and (4.10) still yield (4.11) of course, but the physical interpretation of these definitions in terms of local observations seems less natural.

5. EVOLUTION OF RADIATING DISTORTED BLACK HOLES

The Weyl formalism leads to a simple and explicit description of the behavior of axisymmetric, distorted holes with spherical topology as they evolve by radiating quantum particles.

For the applicability of this description, we shall require (i) that the evolution be sufficiently slow that the hole can be regarded as evolving through a sequence of equilibrium states, (ii) that the evolution be sufficiently fast that instabilities which would tend to move the hole off axis can be ignored,[28] and (iii) that the mass of the hole be sufficiently small that its effects on the external matter can be neglected. By (iii), we may regard the external matter as fixed during the course of the evolution. That is, we have a fixed Weyl background, with potential $\hat{U}$, in which the hole evolves. By (i) and (ii), the hole can be represented, at each instant of time, by a segment H of length $2m$ on the axis of the background, where m is the instantaneous mass of the hole. Since the hole is to be in equilibrium, H will be so located that the potential $\hat{U}$ assumes the same values at its two ends. As the hole evolves by radiating, its various parameters, including m, will in general change. Thus, the segment H, with slowly changing length, will continually readjust its location to maintain equality of $\hat{U}$ at its two ends. In the analogous arrangement of a Newtonian rod of fixed mass density in a background potential, the corresponding behavior would follow from adiabatic invariance of the action.

An example of a background potential $\hat{U}$, produced by external matter perhaps more concentrated in the equitorial plane than on the axis, is shown in Fig. 1. In this example, there is a unique location of the segment H for each value of m: As its length changes, its center will always remain on the dashed curve shown. Thus, we may take u, the common value of $\hat{U}$ at the ends of H, as a function of m, the half-length of H. In this example, $u(m)$ is an increasing function of its argument.

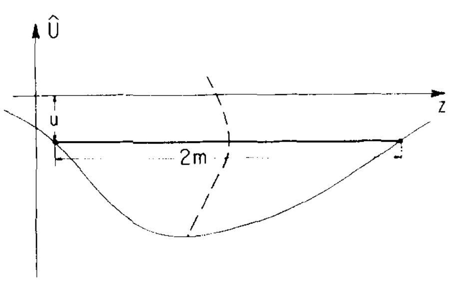

FIG. 1. The equilibrium position of the segment H in a background potential $\hat{U}$. The segment of length $2m$ positions itself such that the potential $\hat{U}$ assumes the same value (denoted u) on its two ends. This determines the function $u(m)$. As m changes, the center of H moves along the dashed curve shown.

In general, from the function $u(m)$, as determined by the background field, together with (3.3) and (4.4), which respectively express the area A of the horizon and the temperature T of the hole in terms of m and u, we obtain

$$\delta m = \tfrac{1}{4}T\left(1 - m\frac{du}{dm}\right)^{-1}\delta A, \tag{5.1}$$

$$\delta T = -\frac{T^2}{4m}\left(1 - 2m\frac{du}{dm}\right)\left(1 - m\frac{du}{dm}\right)^{-1}\delta A. \tag{5.2}$$

Thus, the behavior in time of all the parameters characteristic of the hole is determined from that of any one. But the time rate of change of A is given by the area-decrease formula[27]

$$\frac{dA}{dt} = -\frac{8\pi}{\kappa}\int \langle T_{ab}\rangle t^a t^b\, dA. \tag{5.3}$$

Here $\langle T_{ab}\rangle$ is the renormalized expectation value of the stress energy of the quantum fields, the integral is over a certain cross section of the horizon, and t is Killing time. While the magnitude of the right-hand side of (5.3) is of order AT^4, its detailed evaluation is in general difficult. But there is a simple argument, using the static character, conservation of $\langle T_{ab}\rangle$, and positivity of the energy flux at infinity, which yields that this right-hand side is always nonpositive.[29] Therefore the horizon area (entropy) of the hole decreases monotonically with time in the course of the evolution. The direction of change of m and T are now given by (5.1) and (5.2).

As an example of these remarks, consider the potential $\hat{U}$ shown in Fig. 2. At the location of segment I, $0 < m\, du/dm < \frac{1}{2}$. So, by (5.1) and area decrease, the mass of the corresponding black hole will decrease as it radiates. The segment will therefore become shorter, and so will settle downward into its potential well. Meanwhile, by (5.2) and area decrease, the temperature of the hole will increase. This, of course, is the normal behavior for a Schwarzschild hole. At the location of segment A, on the other hand, $m\, du/dm > 1$. So, by (5.1) the mass of the corresponding hole will increase with time, the segment moving upward in the diagram, while, by (5.2), the temperature is increasing. The behavior of the hole represented initially by segment C is more complicated. There, $\frac{1}{2} < m\, du/dm < 1$, and so the hole will initially have decreasing mass, its segment settling into the potential well, but with temperature also decreasing. The segment, on reaching location D, cannot bifurcate into two segments, one in each potential valley, as is guaranteed by general theorems.[30] So, the segment, still representing a hole with m and T both decreasing, will continue to move downward, approaching location E, where $m\, du/dm = \frac{1}{2}$. There by (5.2), the temperature reaches a minimum, the mass continuing to decrease. So, the segment, representing a hole evolving with decreasing m and increasing T, will continue past location F, where $m\, du/dm = 0$, and then on toward location G. At G, $m\, du/dm = \pm\infty$ (plus from below, minus from above). By (5.1) and (5.2), the segment will move smoothly through location G, with the temperature of the hole continuing to increase, but its mass reaching a minimum there. The hole now grows more massive and hotter, as its segment approaches H, where $m\, du/dm = 1$. This H represents a local minimum of horizon area. There will occur a "runaway" toward H, presumably in finite time, and with rapidly increasing (but finite) m and T. Thereafter, there is no quasistatic equilibrium configuration.

Thus, depending on the behavior of $m\, du/dm$—the values of which are determined solely by the background gravitational field—there can occur evolving black holes with various combinations of increasing or decreasing T or m. We note that these effects will not be seen by the local observers of the previous section, for they, using (4.9) and (4.10), will always find m_{int} decreasing and T_{int} increasing during the evolution.

It seems unlikely that the condition of reasonable external matter will eliminate the effects described above. Indeed, the only obvious constraint on the potential $\hat{U}(z)$ would seem to be that $|m\, d\hat{U}/dz|$, where m measures the size of a hole the potential can accommodate, cannot greatly exceed the order of one. To see this, let M be an effective total mass of the external matter, and L its characteristic distance from the hole. Then

$$\left|m\frac{d\hat{U}}{dz}\right| \lesssim m\left(\frac{M}{L^2}\right). \tag{5.4}$$

But one expects $M/L \lesssim 1$, in order that the external matter not be inside its Schwarzschild radius, and $m/L < A^{1/2}/L \lesssim 1$, in order that the external matter not be in contact with the hole. So, $|m\, d\hat{U}/dz| \lesssim 1$. While this is, of course, a genuine restriction on the external potential $\hat{U}$ (one violated, e.g., near location A in Fig. 2), the behavior of $\hat{U}$ near locations F, G, and H in Fig. 2 shows that there is no corresponding restriction on the values of $m\, du/dm$.

The shape of the horizon during the course of the evolution of the hole can of course be determined from (3.1). The more nearly constant $\hat{U}$ is along the segment, the more nearly spherical the hole. Thus, in the normal situation, such as that of the hole whose segment begins at location I in Fig. 2

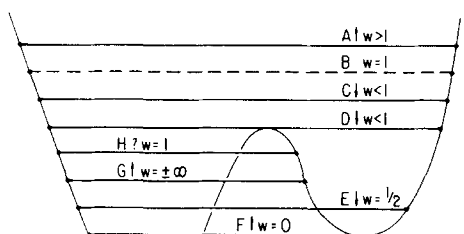

FIG. 2. A potential $\hat{U}$ on the axis that illustrates different possible behaviors of an evaporating distorted Weyl black hole. Various possible line segments H and their corresponding values of $w = m\, du/dm$ are shown on this plot of $\hat{U}$ versus z. The arrows indicate the momentary direction of motion of the segment induced by the Hawking radiation. As described in the text, the segment at I represents a hole that will heat up and lose mass, the segment decreasing its length and settling to the bottom of the well. The segment at A will move upward off the diagram, the hole increasing both its temperature and mass. The segment at C will move through positions D, E, F, and G, with the evolution of the hole becoming nonquasistatic before its segment reaches H. As described in the text, the temperature of the hole at first decreases, reaches a minimum at E, and then increases through the rest of the evolution. The mass decreases through locations D, E, and F, reaches a minimum at G, and thereafter increases.

and thereafter settles into the potential well, the hole becomes more nearly spherical as it evolves. The hole whose segment begins at location A, on the other hand, becomes less spherical. But the argument above suggests that it may not be possible to realize the situation of location A with reasonable external matter. In fact, these observations generalize. One checks from the geometry that the deviation from spherical, measured by the difference between the maximum and minimum of $\hat{U}$ along the segment, can increase during the evolution only when m is increasing and further $d\hat{U}/dz$ at the two ends of the segment have opposite signs. However, from (5.1), this can occur only if $|m\, d\hat{U}/dz|$ exceeds two at at least one end of the segment, which may violate the argument of (5.4). These remarks suggest that there may be a general theorem to the effect that distorted holes in the presence of reasonable external matter must, during the course of their evolution by Hawking radiation, become more spherical.

For the specific heat of the hole we have, from (5.1) and (5.2),

$$C = \frac{\delta m}{\delta T} = -\frac{m}{T} + \frac{2m^2}{T}\frac{du}{dm}. \tag{5.5}$$

For $m\, du/dm > \frac{1}{2}$, this specific heat is positive, in contrast with the usual situation for isolated black holes and for isolated self-gravitating systems in general. The reason for this behavior is the same as the reason why the specific heat of an ideal self-gravitating gas confined to a box can be positive: the action of external forces.[31]

An intriguing question left unanswered here concerns the details of the Hawking radiation from the distorted holes, and in particular the question of whether this radiation carries net linear momentum along the axis of symmetry. For wavelengths short compared to the size of the hole, the radiation should be similar to that from an irregularly shapped black body radiating at a constant temperature from its surface. The resulting radiation has an angular distribution appropriate to the shape of the body, but carries no net linear momentum. But for wavelengths comparable to the size of the hole, the answer is less clear. Unfortunately, the actual motion of the hole itself, as described above, provides no information about the emission of momentum. Consider again the analogous Newtonian arrangement: A rod of fixed mass density in an external potential, which slowly loses mass from its ends and thereby shrinks and settles into the potential well, as in Fig. 1. By adiabatic invariance, no matter how the rod slowly disposes of its mass—by tossing it in one direction or another—the rod will still settle with its center along the dashed line in Fig. 1. The potential soaks up the excess momentum. It would be of interest to have a direct calculation of $\langle T_{ab}\rangle$ for at least some of the distorted holes.

6. GENERAL STATIC BLACK HOLES

We have seen in Sec. 4 that, for distorted Weyl holes with spherical topology, there can be formulated a version of the first law that applies to the system consisting only of the hole itself; and, in Sec. 5, that there can be followed in some detail the quasistatic evolution that results from the Hawking radiation of the hole. It is natural to ask how much of this material can be generalized to the nonaxisymmetric case, i.e., to the class of all static distorted black holes in the background field of an external matter distribution. We shall show in this section that significant generalization is possible.

The relevant parameters for an axisymmetric Weyl hole are its surface gravity and temperature, its horizon area and entropy, its Komar mass, and the effective potential u. Consider now a static, not necessarily axisymmetric, black hole in a static external matter distribution. Which of these parameters are still available in this case? The surface gravity, given by (3.4), is again constant on the horizon, and the temperature T may again be defined in terms of it by (4.2). Indeed, assuming only the presence of a crossing surface, the Gibbons–Perry argument leading to (4.2) applies equally well in the present case. The static Killing field again generates the horizon, and so the area A is again independent of cross section. We may again identify S as $\frac{1}{4}A$, as suggested by the general first law (4.6). The Komar mass m of course makes sense for any static black hole:

$$m = \frac{1}{4\pi}\int_C \epsilon_{abmn}\nabla^m t^n dA^{ab}, \tag{6.1}$$

where t^a is the static Killing field, the integral is over any cross section C of the horizon, and dA^{ab} is the surface element of this cross section.

The difficult parameter is of course the effective potential u. In the Weyl case, u is defined by writing the Weyl potential U as the sum of one potential, U_S, regarded as due to the hole, and a second potential, $\hat{U}$, regarded as due to the external matter, and evaluating $\hat{U}$ at the ends of the segment H that defines the hole. In the absence of axisymmetry, with no Weyl form, we do not of course have such a decomposition. Nonetheless, we may generalize the definition of u as follows. Consider a solution with a static, distorted hole with spherical topology and a distribution of external matter. Imagine building up this solution by the following procedure: First assemble the distribution of external matter, and then take a black hole, initially a Schwarzschild hole far from the matter, slowly move it into the vicinity of the matter, find a position at which the now-distorted hole is in equilibrium, and release it there. In the course of moving the hole, its Komar mass will change from its initial value, m_∞, to some final value, m. We *define* u to be the redshift factor relating these two masses:

$$m_\infty = me^{-u}. \tag{6.2}$$

This formula is suggested, e.g., by the fact that a particle, beginning at infinity with mass m_∞ and moved to an equilibrium position at which $t^a t_a = -e^{2u}$, will there have mass m satisfying (6.2).

At infinity, our hole is Schwarzschild, and so has horizon-area $16\pi m_\infty^2$. But, by (5.3), this area will not change during the slow motion to the equilibrium position. So, from (6.2), we have

$$A = 16\pi m^2 e^{-2u}. \tag{6.3}$$

The temperature T can also be expressed in terms of m and u. Indeed, Bardeen, Carter, and Hawking[25] have shown that the relation $\kappa A/m = 4\pi$, verified in Sec. 3 for the Weyl case, holds for any static black hole. The proof consists of substituting in (6.1) the usual expression for $\nabla^m t^n$ in terms of t^m and the gradient of its norm, using the second expression (3.4), and integrating. From this and (6.3) we obtain

$$T = (8\pi m)^{-1} e^{2u}. \tag{6.4}$$

The local version of the first law for general static holes is now immediate. Take the variation of (6.3) and use (6.4):

$$\delta m = T\delta S + m\delta u. \tag{6.5}$$

In addition, much of the discussion in Sec. 5 of the evolution of the holes can be carried over to the general static case. A hole, initially in the asymptotic region with given mass, will, when moved to its equilibrium position, acquire some values for m and u. So, we may regard u as a function of m. Equations (5.1) and (5.2) again give the changes in m and T during the evolution, and the argument of (5.3) again yields that the area A decreases as a result of the radiation. This is the machinery needed to treat the evolution.

But these results in the general static case do suffer, in comparison with the Weyl case, from significant limitations. For a distorted Weyl hole, we have a mathematically natural prescription for extracting from the Weyl potential U a background potential $\hat{U}$. Therefore u is determined, say as a function of m, immediately from the background gravitational field, with the result that the local first law and the discussion of evolution are made explicit. In the general static case, by contrast, while we do have an opertional definition of u, and exactly the same formulae relating T, A, m, and u, we do not have the same direct access to the values of u. As an example of this difference, recall that we showed in the Weyl case, in Sec. 4, that u must be nonpositive under the strong energy condition on the external matter. It is by no means clear that any similar result holds in the general static case.

7. DISCUSSION

Static, axisymmetric black holes are a remarkably simple class of solutions of Einstein's equation. They come in just two topological types—spherical and toroidal—each with its own global structure. Their local properties are determined by a single solution of Laplace's equation, while many of their physically interesting characteristics (e.g., horizon area, surface gravity) are expressed in terms of just two parameters, m and u. Despite this simplicity, there is a great variety of Weyl black hole solutions. They can thus be used to illustrate and formulate thermodynamic and quantum behavior in a way not possible for the Kerr family of isolated black holes.

It would be of interest to see to what extent the results obtained here can be generalized to other classes of black holes. Dynamic holes would seem to be too difficult for immediate investigation. The time-independent holes can be classified according to whether they are static or stationary (i.e., whether the time symmetry is surface orthogonal), and whether they are rotating or nonrotating (i.e., whether the time symmetry generates the horizon). Whereas all static holes must be nonrotating, the stationary holes include some (all axisymmetric[32]) that are rotating, and, apparently, some that are not.[33] A very special class of stationary, rotating black holes can be obtained by taking the present Weyl class of local black holes, choosing for the "time symmetry" a suitable linear combination of t^a and φ^a, and then extending to achieve asymptotic flatness with this time symmetry an asymptotic time translation.

What, in analogy with the Weyl case, are the possible topologies for cross sections of the horizons of these more general black holes? If the external matter satisfies an energy condition, then in all cases only spherical topology is possible, as Hawking has shown.[15] Suppose, however, that this energy condition were relaxed. Then, for axisymmetric holes—a class that includes all rotating holes as well as our Weyl examples—the only possibilities are spherical and toroidal, by the argument of Appendix B. But for holes nonaxisymmetric and with no energy condition, are more complicated topologies possible? Our consideration of the Weyl case suggests that, should such holes exist, the external distorting matter would have to be very carefully constructed (in addition to its having negative energy). For the Weyl toroidal holes, for example, there must always be external matter (or singular behavior) extending "through the doughnut."[34] Is there any analogous result for more complicated topologies? Suppose, under such an arrangement, the matter were slowly moved from the vicinity of the hole to distant regions. How would the hole, which could not, presumably, permit this to happen while retaining its horizon-topology, react? Similarly, what would happen if a spinning gyroscope were dropped into a hole with other than spherical or toroidal topology? The hole could not become rotating consistent with its horizon-topology. To what equilibrium state would it finally settle, and how would it radiate to achieve this state?

Space–times with distorted black holes provide useful examples for the formulation and study of the laws of black-hole thermodynamics. As we saw in Sec. 6, thermodynamic laws can be formulated with general static black holes, not only for the total system of hole plus external matter, but also for the black hole considered as a single system. Can similar laws be formulated for stationary, axisymmetric black holes? The two key starting points in Sec. 6 were the relation between m, κ, and A and the operational definition of the potential u, both in the general static case. The former has been generalized, including angular velocity and angular momentum, to stationary holes.[25] But what of the latter? What is needed is the proper definition of the work done on the black hole by axisymmetric deformations of the external matter. The static case suggests that some insight into this may be obtained by studying the changes in the parameters describing the hole as it is lowered axisymmetrically into an axisymmetric distorting system.

In addition to these issues, which involve generalizing Weyl results, there remain a number of interesting questions concerning the Weyl black holes themselves. We mention a few.

In Sec. 5, we discussed the quasistatic evolution of a single radiating Weyl black hole in a background of distorting matter. One might consider the case of two or more black holes evolving together. Each hole will then feel not only the field of the external matter, but also the evolving fields of the other black holes. Neglecting the absorption of Hawking radiation by the holes, this problem should be soluble by the methods of Sec. 5.

It would further be of interest to settle the question raised in Sec. 5 as to whether a distorted black hole can radiate linear momentum. A related issue, also raised in Sec. 5, is whether a static black hole always evolves in its static background in such a way as to reduce its spherical symmetry. A broader question concerns the evolution of isolated but momentarily distorted black holes. Do such holes radiate in such a way as to increase or descrease their distortion? If the distortion increases and the hole radiates momentum, could there result a runaway effect? Or, are there general results which forbid this?

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APPENDIX A: THE WEYL CHARACTERIZATION

Essentially every static, axisymmetric solution of Einstein's equation can be written in Weyl form, (2.3), and this characterization is essentially unique. The details follow.

Let (M,g_{ab}) be a solution of Einstein's equation, with zero stress-energy and with commuting, orthogonal, surface-orthogonal Killing fields, t^a (complete and everywhere timelike) and φ^a. Let there exist an orientable spacelike slice S in this space-time, everywhere orthogonal to t^a and such that every point of M is reached in one and only one way by a t-orbit from a point of S. Then $M = S\times\mathbb{R}$. Define smooth scalar fields U and r^2 on S by the formulae

$$e^{2U} = -t^a t^b g_{ab}, \quad r^2 e^{-2U} = \varphi^a\varphi^b g_{ab}. \tag{A1}$$

Let X be the scalar field on S given by

$$\begin{aligned} X &= e^{-2U} g^{ab}(\nabla_a r)(\nabla_b r) \\ &= \tfrac{1}{2}(\nabla_a\varphi_b)(\nabla^a\varphi^b) + e^{-2U}\nabla_a U\nabla^a(r^2) \\ &\quad - r^2 e^{-2U}(\nabla_a U)(\nabla^a U), \end{aligned} \tag{A2}$$

where ∇_a is the derivative operator of (M,g_{ab}). The second expression follows from the first, expanding the derivative of φ^a in terms of its norm and using (A1). This X is nonnegative, by the first expression, and smooth, by the second.

Were our metric in Weyl form, then, from (2.3) and the first expression (A2), we would obtain $X = e^{-2V}$. Hence, the following two properties would hold: (i) $X = 1$ at all axis points (where $r = 0$), and (ii) X is strictly positive. But the converse is also true. Let these two properties hold. Then (ii) implies that the V defined by $X = e^{-2V}$ is smooth, and (i) that this V vanishes on the axis. Hence, defining h^{ab} on S by (2.3), our metric would be in Weyl form. Furthermore, this representation would be unique, except for the freedom to rescale φ^a by a constant in those situations in which there is no axis. [When there is an axis, this freedom is lost, by condition (i).] There remains, therefore, only the issue of when conditions (i) and (ii) can be achieved.

Condition (*i*): First note that X cannot vanish at any axis point, for otherwise, by the second expression (A2), both φ^a and its derivative would vanish at a point, implying $\varphi^a = 0$ everywhere. Furthermore, taking the gradient of the second expression (A2), we find that the gradient of X vanishes on the axis. Thus, by rescaling φ^a by a constant, we can always achieve $X = 1$ on any one connected part of the axis. Unfortunately, the axis will in general consist of more than one connected component, and it is not true in general that X assumes the same constant value on each component. (When not, then the metric has no Weyl form. Note that this is a quite different issue than the usual one of "wire singularities.") But constancy of X on the entire axis does hold in cases of interest, e.g., whenever all closed φ^a-orbits have the same period, and whenever φ^a is complete.

Condition (*ii*): It is a consequence of Einstein's equation that r is harmonic in local 2-surfaces in S orthogonal to φ^a. However, X vanishes where and only where the gradient of r vanishes [first expression, (A2)], which in turn is where and only where the gradient of the corresponding complex analytic function vanishes.[35] Therefore, either $X = 0$ everywhere, or else X has at most isolated zeros. The case $X = 0$ everywhere leads to flat space–time: Writing out explicitly the vanishing of the projection of the Ricci tensor into the 2-planes orthogonal to the Killing fields, and using $X = 0$, one obtains $U =$ const. But this implies (since t^a is surface orthogonal) that t^a is a constant vector field in the space-time, and so (equating to zero the second derivative of t^a) that $C_{abcd}t^d = 0$, where C_{abcd} is the Weyl tensor, and so (since t^a is nowhere null) that $C_{abcd} = 0$. Thus certain representations of flat space-times as "static and axisymmetric" cannot be written in Weyl form.

The case of isolated zeros of X, as it turns out, can occur. An example (obtained by merely repeating the standard Weyl construction, but without introducing an r coordinate) follows. In a neighborhood of the origin of the flat 2-plane with Euclidean coordinates x,y, let r be the (harmonic) function $2 + x^2 - y^2$, and let U be any solution of $\mathscr{D}^2 U + r^{-1}(\mathscr{D}_a U)(\mathscr{D}^a r) = 0$ having gradient (0,1) at the origin, where $\mathscr{D}_a$ is the flat derivative operator. Now consider the equation

$$\begin{aligned} \mathscr{D}_a V = (\mathscr{D}_m r\mathscr{D}^m r)^{-1}[2m\mathscr{D}_a U\mathscr{D}_b U \\ - r\mathscr{D}^m U\mathscr{D}_m U g_{ab} + \mathscr{D}_a\mathscr{D}_b r]\,\mathscr{D}^b r. \end{aligned} \tag{A3}$$

Away from the origin, the curl of the right side of (A3) vanishes identically, and, taking a divergence there, we have $\mathscr{D}^2 V = -\mathscr{D}_a U\mathscr{D}^a U$. On approaching the origin, $\mathscr{D}_m r\mathscr{D}^m r = 4(x^2 + y^2)$ vanishes quadratically. But both the expression in square brackets in (A3) and the $\mathscr{D}^b r$ vanish at the origin, by our choices of r and U, and so the right-hand side of (A3) remains bounded at the origin. It follows[36] that V satisfying (A3) is smooth, including at the origin. The metric is now given by

$$ds^2 = e^{+2V-2U}(dx^2 + dy^2) + r^2 e^{-2U}d\varphi^2 - e^{2U}dt^2. \tag{A4}$$

The isolated zero of X is of course at the origin. These solutions are apparently new, but just barely so as they are Weyl solutions, and hence known, almost everywhere.

Thus, except for certain solutions with anomalous global t-behavior, certain with anomalous global axis-behavior, certain representations of flat space-time, and certin local solutions of the type (A4), all static, axisymmetric solutions are Weyl.

APPENDIX B: BLACK HOLE CANDIDATES

Let the Weyl solution (2.3) associated with (S,h_{ab},U,V) be a local black hole in the sense of Sec. 2. We show that this solution must, at least in a neighborhood of the horizon, coincide with one of the local Weyl holes listed in that section.

First note that a cross section of the horizon must be a compact, orientable two-dimensional manifold with positive-definite metric and nonzero Killing field φ^a. Since the sum of the indices of the zeros of φ^a must be the Euler number of this cross section, and since, by the Killing character, each index must be $+1$, there are just two possibilities: a topological sphere (two zeros of φ^a) and a topological torus (no zeros). We first sketch the topological structure of each possibility.

In the spherical case, the orbits of φ^a must, from their behavior near a zero, all be closed circles of the same period. Rescale φ^a so that the period is 2π. The axis in the external region must meet this cross section in just the two zero-points. In a neighborhood of the horizon, S must be topologically $S^2\times\mathbb{R}$. Further, as we showed in Sec. 2, r^2 must vanish on the horizon. Thus, as $r^2\to 0$, the ends of the cylinders of constant r in S must collapse down to an axis, their centers to the horizon. One shows from this that (S,h_{ab},φ^a) must be of the form $S=\bar{S}-H$, where H is a segment of the axis in Euclidean 3-space with axial Killing field φ^a, and $\bar{S}$ is an open neighborhood of this H. The Weyl potential U must of course be smooth on S, but may be singular in $\bar{S}$ at H.

In the toroidal case, S must, in a neighborhood of the horizon, be topologically $S^1\times S^1\times\mathbb{R}$, with the $S^1\times S^1$'s the surfaces of constant r. There can be no axis in such a neighborhood. If the orbits of φ^a are closed circles on these toruses, they must all have the same period, in which case we may rescale φ^a so that the period is 2π. If the orbits are not closed, then each orbit is dense in its torus, in which case we may choose a new axial Killing field φ^a which does have closed orbits. The angle α of Sec. 2 is defined by starting at any point p of a torus, moving within that torus orthogonally to φ^a until reaching the point, q, at which the φ^a-orbit through p is next encountered, and setting α the φ-angle between p and q on this orbit. Thus, in S we have flat tori of constant r, each with Killing field φ^a of period 2π, with these tori converging, as $r\to 0$, to the horizon. That is, we have $S=\bar{S}-H$ as in Sec. 2, with, again, U smooth on S but in general singular on H in $\bar{S}$.

The rest of the argument is local, dealing with the detailed behavior of U near H. The idea is to show that the presence of the Killing fields and a horizon imply that U must go "like $\ln r$" near the horizon, whence $U-U_S$ or $U-U_T$ must be smooth at H.

Since we have a local black hole, the norms of the two Killing fields, e^{2U} and r^2e^{-2U}, must be bounded near H. That is, for some constant c we have

$$\ln r - c \leqslant U \leqslant c \tag{B1}$$

in a neighborhood of H. But these bounds on U imply in turn that U is a distribution on S. Thus $\delta = D^2U$ is also a distribution, and, by (2.1), one with support in H. The next step is to show that the distribution δ is that of a line-density. Let f be any smooth, nonnegative function with compact support in S. Then we have

$$\begin{aligned}\delta(f) &= \int_{\bar{S}}(D^2f)U\,dV = \lim_{x\to 0}\int_{r\geqslant x}(D^2f)U\,dV\\ &= \lim_{x\to 0}\int_{r=x}(fD_aU - UD_af)\,d\Sigma^a\\ &= \lim_{x\to 0}\int_{r=x}D_a(fU)\,d\Sigma^a\\ &= \lim_{r_0\to 0} r_0^{-1}\int_0^{r_0}dx\int_{r=x}D_a(fU)\,d\Sigma^a = \lim_{r_0\to 0}\int_{r=r_0}fU\,dA,\end{aligned} \tag{B2}$$

where the first step is the definition of δ, the third follows by integration by parts, using (2.1), the fourth from the fact that the limit of the integral of the second term in the previous step vanishes, from (B1), and the sixth from performing the x integral. But this last expression for $\delta(f)$, together with the second inequality (B1), implies the second inequality of

$$2\pi\int_H f\,dz \leqslant \delta(f) \leqslant 0. \tag{B3}$$

The first inequality of (B3) follows by repeating this argument, replacing U by $\ln r - U$. But it is not difficult to show that a distribution δ with support in H and satisfying (B3) for every nonnegative test function f must be of the form

$$\delta(f) = 2\pi\int_H f\rho\,dz \tag{B4}$$

for some integrable function ρ on H with $0\leqslant\rho\leqslant 1$. Thus, we have shown so far that the source for U must be a line density on H, with strength everywhere between zero and one.

We next show that the strength must be one. Write out, from $D^2U=\delta$, U as the sum of the inhomogeneous solution obtained using the Green's function and ρ and a homogeneous solution on S. There follows an expression for $D_a U$, and from this that, for almost all points p of our segment H, the limit, along an integral curve of $-D^ar$ approaching p, of $w(r) = r\,\partial U/\partial r$ is $\rho(p)$, and of $r\,\partial U/\partial z$ is zero. (The homogeneous solution does not contribute in these limits.) But this implies, from (2.2), that V approaches $\rho(p)^2\ln r$, in the sense that the quotient approaches one, and that U approaches $\rho(p)\ln r$. Now consider

$$\begin{aligned}&(\nabla_a t_b)(\nabla_c t_d)g^{ac}g^{bd}\\ &\quad = e^{4U-2V}(D_aU)(D_bU)h^{ab} \geqslant r^{-2}e^{4U-2V}w^2.\end{aligned} \tag{B5}$$

Since we have a local black hole, the left-hand side must be bounded near H, and so therefore must the right-hand side. For $0<\rho(p)<1$, this right side approaches $\rho(p)r^{-2[\rho(p)-1]^2}$, which is not bounded. For $\rho(p)=0$, boundedness requires that $r^{-1}w^2$ be bounded, which contradicts the property that $U=\int w/r$ approach $-\infty$ at H. So, $\rho(p)=1$ almost everywhere, i.e. (since only integrals of ρ count) everywhere.

Now set $U=U_S+\hat{U}$ in the spherical case (H a line-segment), and $U=U_T+\hat{U}$ in the toroidal (H a circle), with U_S and U_T as given in Sec. 2. Then, since the strength of the source of U is one—precisely the strength of the sources of

U_S and U_T—$\hat{U}$ is a distributional solution of Laplace's equation, with zero source everywhere on $\bar{S}$. It follows that U is smooth.

Thus, we recover both the topology of (S, h_{ab}, φ^a) and the form of U given in Sec. 2.

[1]For recent reviews see the articles by B. Carter, S. Chandrasekhar, G. Gibbons, and S. W. Hawking in *General Relativity: An Einstein Centenary Survey*, edited by S. W. Hawking and W. Israel (Cambridge U. P., Cambridge, 1979).

[2]See, for example, the article by S. Chandrasekhar in Ref. 1.

[3]See L. Smarr, in *Sources of Gravitational Radiation*, edited by L. Smarr (Cambridge U. P., Cambridge, 1979).

[4]W. Israel, Phys. Rev. **164**, 1776 (1967); B. Carter, Phys. Rev. Lett. **26**, 331 (1971); S. W. Hawking, Commun. Math. Phys. **25**, 152 (1972); S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of Space-time* (Cambridge U. P., Cambridge, 1973); D. C. Robinson, Phys. Rev. Lett. **34**, 905 (1975).

[5]H. Weyl, Ann. Phys. **54**, 117 (1917); J. L. Synge, *Relativity: The General Theory* (North Holland, Amsterdam, 1964), p. 309.

[6]W. Israel and K. A. Khan, Nuovo Cimento **33**, 331 (1964).

[7]L. A. Mysak and G. Szekeres, Can. J. Phys. **44**, 617 (1966).

[8]W. Israel, Lett. Nuovo Cimento **6**, 267 (1973).

[9]P. C. Peters, J. Math. Phys. **20**, 1481 (1979).

[10]See, e.g., G. Erez and N. Rosen, Bull. Res. Council Israel **8F**, 47 (1959).

[11]B. Carter, in *Black Holes*, edited by C. DeWitt and B. DeWitt (Gordon and Breach, New York, 1973).

[12]This condition is needed to ensure that V, satisfying (2.2), can be made to vanish simultaneously on both connected components of the axis. This is seen most easily by integrating (2.2) along a line segment parallel to, and near H.

[13]To see that the resulting $\hat{U}$ will have no singularities, first note, from (2.5), that extension is necessary only to the region $z^2 - m^2 \leqslant r^2 \leqslant 0$. But, by (2.1), $\hat{U}$ satisfies a linear hyperbolic equation in this region, while the segment $-m < z < m$, $r^2 = -\epsilon$ (with ϵ small and positive) is a Cauchy surface for this region.

[14]This argument fails at the crossing point at the center of the Kruskal diagram, where the gradient of e^{2U_S} does vanish. But $e^{2\hat{U}}(1 - e^{4\hat{U} - 4u - 2\hat{V}})$ vanishes one order faster there, with the result that all terms in (2.8) again remain smooth on this 2-sphere.

[15]S. W. Hawking, Commun. Math. Phys. **25**, 152 (1972).

[16]The singular regions in Peters' example will thus have been filled in by matter in the present extensions.

[17]J. Bekenstein, Phys. Rev. D **7**, 2333 (1973); D **9**, 3292, (1974); D **12**, 3077 (1975).

[18]S. W. Hawking, Nature **248**, 30 (1974); Commun. Math. Phys. **43**, 199 (1975).

[19]We consider only the case of a single black hole. For multiple black holes, each will have its own characteristic temperature, and so thermal equilibrium will not in general be possible.

[20]G. W. Gibbons and M. J. Perry, Phys. Rev. Lett. **36**, 283 (1976); Proc. Roy. Soc. London Ser. A **358**, 467 (1978).

[21]G. W. Gibbons and S. W. Hawking, Commun. Math. Phys. **66**, 291 (1979).

[22]Here, as throughout, we employ units in which $G = c = \hbar = k = 1$.

[23]R. C. Tolman and P. Ehrenfest, Phys. Rev. **36**, 1791 (1930).

[24]Contrast this situation with that of Newtonian gravitational theory. There, the kinetic energy of a particle also changes as it moves, but now by addition of a term (rather than multiplication by a factor) depending on the initial and final position. As a result, the temperature as measured by a local thermometer is constant throughout a Newtonian gravitating system in thermal equilibrium.

[25]J. M. Bardeen, B. Carter, and S. W. Hawking, Commun. Math. Phys. **31**, 161 (1973).

[26]In the Weyl case, constancy of the surface gravity is equivalent to constancy of $\hat{U} - \frac{1}{2}\hat{V}$ on the horizon.

[27]S. W. Hawking and J. B. Hartle, Commun. Math. Phys. **27**, 283 (1972).

[28]It is clear physically that all the solutions under discussion here are unstable to perturbations under which the black hole is displaced off the axis of symmetry. The hole will continue to fall toward the attracting external matter.

[29]P. Candelas, Phys. Rev. D **21**, 2185 (1980).

[30]S. W. Hawking, Phys. Rev. Lett. **26**, 1344 (1971).

[31]In fact, (5.5) is analogous, term for term, to the expression for the specific heat of an ideal gas in an external gravitational potential U: $C = -K/T + \int d^3x\,(d\rho/dT)\mathbf{x}\cdot\mathbf{D}U$, where K is the kinetic energy and ρ the mass density. This relation follows easily from the virial theorem. We are indebted to H. Kandrup for discussion of this point.

[32]Ref. 15, and S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of Space-Time* (Cambridge U. P., Cambridge, 1973).

[33]For such a hole, the Killing field of time symmetry would have to generate the horizon, but be non-hypersurface-orthogonal outside. Such a hole might be produced by placing a nonrotating hole in the gravitational field of a nonaxisymmetric, stationary, nonstatic matter distribution, e.g., the field of a garden hose twisted into a nonaxisymmetric shape with water flowing through it at constant speed. This arrangement would not seem to violate the theorem of Ref. 32.

[34]One sees this as follows. The Weyl metric is applicable until matter is encountered. Suppose that the matter "does not extend through the doughnut" in the sense that, restoring H as an axis in S to obtain $\bar{S}$ as in Sec. 2, this circle H can be contracted to a point in $\bar{S}$. We obtain a contradiction. Denote by z^a the unit tangent vector to the curve H, so, since H is a geodesic, z^a is constant on H. On each successive closed curve γ obtained during the contraction of H, let z^a be that given by parallel transport in the flat space $(\bar{S}, h_{ab})$ from the nearby preceding curve. Then, by parallel transport, $\int_\gamma z_a \, dl^a$ does not change as γ varies from one curve to the next. But this is a contradiction, for the integral is $2m$ for the initial curve H, and zero for the final curve at a point.

[35]This argument is due to Greg Horndeski.

[36]G. B. Folland, *Introduction to Partial Differential Equations* (Princeton U.P., Princeton, NJ, 1976), Chap. 6.

ERRATA

Erratum: Inverse scattering. II. Three dimensions [J. Math. Phys. 21, 1698 (1980)]

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I am indebted to Professor Y. Saitō for pointing out to me that the equation four lines from the bottom of the left-hand column of p. 1713 is in error and should be replaced by

$$V'(x,y,\theta) = \frac{(\theta - \hat{y}\theta\cdot\hat{y})\cdot\nabla V(x+y)}{1-(\theta\cdot\hat{y})^2}.$$

As a result the proof of Lemma 3.2 is invalid. A modification of this proof by means of Hölder's inequality leads to the following replacement of Lemma 3.2: If the assumptions stated in Lemma 3.2 are made, and in addition it is assumed that $\exists C_1$ and μ such that for all $k\in\mathbb{R}^3$

$$|\tilde{V}(k)| \leqslant C_1(\mu^2 + |k|^2)^{-1},$$

where $\tilde{V}$ is the Fourier transform of V, then for all $p>4$, $\exists C_2$ such that for all $f\in L^p(S^2)$

$$\int_{-\infty}^{\infty} dk\, k^2 \| A_k f \|_p^2 < C_2 \| f \|_p^2,$$

where $\|\cdot\|_p$ is the L^p norm.

This form of Lemma 3.2 (and its corresponding change in the corollary on p. 1704) suffices for all subsequent results.

Erratum: Inverse scattering. III. Three dimensions, continued [J. Math. Phys. 22, 2191 (1981)]

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The lower limits on the k-integrals in the equations on lines 7 to 10 from the bottom of the right-hand column on p. 2192 should all be $-\infty$. Equaticn (A3) is valid for $0<\alpha<1$. The equation four lines below (A3) should read

$$(\theta' - \theta'')^2(\theta - \theta'')^2 = (2 - |\theta + \theta'|u)^2 - |\theta - \theta'|^2(1-u^2)\cos^2\phi,$$

and similarly in the integral in the next line. In line 6 from below in the same column, it should be $O(|a^2-1|^{\alpha/2-1})$, and in line 4 from below, $a^2 \geqslant b^2$.

Erratum: On the existence of simultaneous synchronous coordinates in spacetimes with spacelike singularities [J. Math. Phys. 22, 2659 (1981)]

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In the publication of our paper, several paragraphs in Sec. IV were printed twice, with the second printing corresponding to the uncorrected galley proofs and thus containing some minor errors. Therefore, the material beginning on line four of the first column of p. 2664 and ending on the fifth line below Eq. (4.6) on the second column of that page should be deleted.