Properties of Poincaré generating functions for polynomial covariants (tensors)

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(Received 21 December 1983; accepted for publication 1 June 1984)

We show that irreducible polynomial covariants (tensors) based on a given irreducible representation of a finite group must have a definite p-phase, i.e., degree modulo p, where p is the order of the center of the image of the group. We also show that the numerator of the Poincaré function is often a polynomial symmetric around a given degree and we derive several interesting properties of the Poincaré function.

PACS numbers: 02.20 + b, 02.30. + g, 11.15. − q, 61.50.Em

I. INTRODUCTION

In many areas of physics one is faced with a problem of describing or constructing irreducible polynomial covariants (tensors) based on a given representation of a physical group G. For example, in the Landau theory of phase transitions[1,2] and in the Higgs mechanism of gauge theories[3,4] one requires construction of the invariants and the vector fields.[5] On the other hand, a need for constructing covariants for crystallographic point groups was realized by Bethe half a century ago[6]: these are the crystal harmonics, a generalization of spherical harmonics, the well-known covariants of O(3).

The above general problem can be formulated more precisely as follows. Let χ be a unitary character (representation) of a compact group G acting on a vector space V over the field $\mathbb{C}$ of complex numbers ($V \sim \mathbb{C}^{\dim \chi}$). Let, furthermore, $\mathbb{C}[V]$ be the ring of complex polynomials on V. As an infinite-dimensional vector space, $\mathbb{C}[V]$ can be decomposed into the sum of subspaces $\mathbb{C}[V]^m$ of homogeneous polynomials of degree m. The unitary action of G on V induces a linear action on $\mathbb{C}[V]$ for which $\mathbb{C}[V]^m$ are invariant subspaces. Each $\mathbb{C}[V]^m$ can, thus, be decomposed into isotypical invariant subspaces $\mathbb{C}[V]^m_{\hat{\alpha}}$ which carry the irreducible representations $\hat{\alpha}$ of G. The multiplicity of $\hat{\alpha}$ in $\mathbb{C}[V]^m_{\hat{\alpha}}$, denoted $\mu_m(\hat{\alpha},\chi)$, is the number of times $\hat{\alpha}$ occurs in $\chi^{[m]}$, the mth symmetrized power of χ. Therefore, the problem of describing $\mathbb{C}[V]$ reduces to (i) finding the multiplicity $\mu_m(\hat{\alpha},\chi)$ and (ii) finding $\mu_m(\hat{\alpha},\chi)$ linearly independent sets of $\dim \hat{\alpha}$ homogeneous polynomials of degree m, each set forming a basis for $\hat{\alpha}$ (see Refs. 7 and 8).

While the second problem may be answered using the projection operator techniques, the first problem is solved by calculating the Poincaré series. It is a formal power series

$$P(\hat{\alpha},\chi;t) = \sum_{m=0}^{\infty} \mu_m(\hat{\alpha},\chi) t^m. \tag{1}$$

For finite groups, with which we will be concerned in the rest of this paper, $P(\hat{\alpha},\chi;t)$ may be shown to converge for sufficiently small t to a rational function

$$P(\hat{\alpha},\chi;t) = N(\hat{\alpha},\chi;t)/D(\chi;t), \tag{2}$$

where N and D are polynomials in t (see Ref. 8). In fact, it can be shown[8] that they have a general form

$$D(\chi;t) = \prod_{i=1}^{\dim \chi} \chi\,(1 - t^{d_i(\chi)}),\ d_i \geqslant 1, \tag{3}$$

and

$$N(\hat{\alpha},\chi;t) = \sum_{j=1}^{l(\hat{\alpha},\chi)} t^{\delta_j(\hat{\alpha},\chi)},\ \delta_j \geqslant 0. \tag{4}$$

The forms Eqs. (2)–(4) betray a deeper structure of $\mathbb{C}[V]$. They are consequences of the following important facts.[8]

Theorem 1.1: For a given χ, the following hold.

(a) There are precisely $\dim \chi$ algebraically independent G-invariant homogeneous polynomials $\theta_i \in \mathbb{C}[V]$, $\deg \theta_i = d_i$, $i = 1,2,...,\dim \chi$, such that $\mathbb{C}[V]$ is a *free* module over the polynominal ring $\mathbb{C}[\theta_1,\theta_2,...,\theta_{\dim \chi}]$.

(b) Each $\mathbb{C}[V]_{\hat{\alpha}} \equiv \oplus_{m=0}^{\infty} \mathbb{C}[V]^m_{\hat{\alpha}}$ is a free $\mathbb{C}[\theta_1,\theta_2,...,\theta_{\dim \chi}]$ module.

(c) The action of G on the quotient ring $\mathbb{C}[V]/(\theta_1,...,\theta_{\dim \chi})$ is isomorphic to κ times the regular representation of $\chi(G)$ [i.e., $l(\hat{\alpha},\chi) = \kappa(\chi)\dim \hat{\alpha}$, in Eq. (4)] with the basis covariants being homogeneous of degree $\delta_j(\hat{\alpha},\chi)$.

That is, for each irreducible representation $\hat{\alpha}$ there are precisely $l(\hat{\alpha},\chi) = \kappa(\chi)\dim \hat{\alpha}$ independent basic $\hat{\alpha}$-covariant homogeneous polynomial fields $b^{\hat{\alpha}}_j$, $\deg b^{\hat{\alpha}}_j = \delta_j(\hat{\alpha},\chi)$, $j = 1,2,...,l(\hat{\alpha},\chi)$, such that every $\hat{\alpha}$-covariant polynomial field $v_{\hat{\alpha}}$ can be decomposed as

$$v_{\hat{\alpha}} = \sum_{j=1}^{l(\hat{\alpha},\chi)} q_j b^{\hat{\alpha}}_j, \quad q_j \in \mathbb{C}[\theta_1,\theta_2,...,\theta_{\dim \chi}], \tag{5}$$

where the coefficients q_j are uniquely determined by v_α. [By $\hat{\alpha}$ covariant we mean a map $v_{\hat{\alpha}}: V \to \mathbb{C}^{\dim \hat{\alpha}}$ such that for every $g \in G$ one has $v_{\hat{\alpha}} \circ \hat{\chi}(g) = \hat{\alpha}(g) \circ v_{\hat{\alpha}}$.]

The Poincaré series have often been calculated. Most often physicists were concerned with the invariants and they have calculated corresponding Poincaré series (also called Molien functions[9]) for irreducible representations of three-dimensional point groups[10–13] and for some irreducible representations of a space group.[14] A general procedure for calculating Molien functions for irreducible representations of space groups has also been developed.[14,15] Furthermore, Poincaré series for covariants of ordinary[16–19] and spin representations of three-dimensional point groups,[20] as well as

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 0022-2488/84/123363-04$02.50

for magnetic point groups,[21] have been calculated. The Poincaré series (as well as some other interesting generating functions) have also been calculated for representations of compact Lie groups[22] and the topic has been reviewed recently.[23]

However, in most of the above-cited work very little attention is paid to general relations among Poincaré series of a group.[24] For example, in Ref. 17 it is pointed out that for irreducible characters $\hat{\alpha}$ and $\hat{\chi}$, the series must satisfy

$$\sum_{\hat{\alpha}} \dim \hat{\alpha}\, P(\hat{\alpha},\hat{\chi};t) = (1-t)^{-\dim \hat{\chi}}, \tag{6}$$

but there remain unanswered some obvious questions. For example: Is it an accident that very often for a group and a given $\hat{\chi}$ the polynomials $N(\hat{\alpha},\hat{\chi};t)$ are symmetrical around a given power (which depends only on $\hat{\chi}$)? Or when the above is not the case, like for the Γ_2 and Γ_3 representations of the tetrahedral group T, is there any significance in the fact that there are some simple relations among the series [e.g., $N(\Gamma_1,\Gamma_3;t) = t^2 N(\Gamma_3,\Gamma_2;t^{-1})$ for T, in the notation of Ref. 17]? Or why for the vector representation of the full cubic group O_h all the series are *either* even or odd? The remainder of this short paper is concerned with precisely such questions.

It will be first shown in the next section how the the Poincaré series for reducible representations can be calculated from the series for irreducible ones using the Clebsch–Gordan coefficient. From thereon only the series for irreducible characters will be considered. First, the results which answer the first two of the above-mentioned questions will be derived. Then, some simple results based on the center of G and on the kernel of $\hat{\chi}$ will be deduced. Sec. III will be concerned with some deeper results based on a notion of p-phase of $\hat{\alpha}$ relative to $\hat{\chi}$.

II. SIMPLE RESULTS

The Poincaré series [Eq. (1)] can be generalized to the case when both representations are reducible: $\alpha = \alpha_1 \oplus \alpha_2$ and $\chi = \chi_1 \oplus \chi_2$. In that case $\mu_m(\alpha,\chi)$ is the intervening number for α and $\chi^{[m]}$,

$$\mu_m(\alpha,\chi) = \langle [\operatorname{tr} \alpha(g)]^* [\operatorname{tr} \chi^{[m]}(g)] \rangle, \tag{7}$$

where we used $\langle \cdots \rangle$ to denote the group average. Clearly, $\operatorname{tr}(\alpha_1 \oplus \alpha_2) = \operatorname{tr}\alpha_1 + \operatorname{tr}\alpha_2$ and $\mu_m(\alpha,\chi) = \mu_m(\alpha_1,\chi) + \mu_m(\alpha_2,\chi)$. Consequently,

$$P(\alpha_1 \oplus \alpha_2,\chi;t) = P(\alpha_1,\chi;t) + P(\alpha_2,\chi;t), \tag{8}$$

and it suffices to consider irreducible $\alpha = \hat{\alpha}$ (see Ref. 25).

On the other hand, it is well known[8] that $\operatorname{tr}\chi^{[m]}$ is generated by $\det(1-\mathrm{t}\chi)^{-1}$ and

$$P(\hat{\alpha},\chi;t) = \langle \operatorname{tr} \hat{\alpha}(g)^* \det[1-\mathrm{t}\chi(g)]^{-1} \rangle. \tag{9}$$

Using this equation and $\det(1-t\chi) = \det(1-\mathrm{t}\chi_1)\det(1-t\chi_2)$ for $\chi = \chi_1 \oplus \chi_2$, we write

$$P(\hat{\alpha},\chi;t) = \langle \langle [\operatorname{tr} \hat{\alpha}^*(g)] \det[1-\mathrm{t}\chi_1(g)]^{-1} \times \delta_{gg'} \det[1-t\chi_2(g')]^{-1} \rangle \rangle, \tag{10}$$

with an obvious notation. We define $\delta_{gg'} = \delta_{g'g}$ by

$$\langle \delta_{gg'} F(g') \rangle = F(g), \tag{11}$$

for every function $F(g)$ defined on the conjugacy classes of G. Owing to the orthogonality relations among irreducible unitary characters of G, $\delta_{gg'}$ can be represented as

$$\delta_{gg'} = \sum_{\hat{\beta}} [\operatorname{tr} \hat{\beta}^*(g)][\operatorname{tr} \hat{\beta}(g')]. \tag{12}$$

Substituting this expression into Eq. (10) and using the Clebsch–Gordan series, $\hat{\gamma} \times \hat{\beta} = \Sigma_{\hat{\alpha}} C^{\hat{\alpha}}_{\hat{\gamma},\hat{\beta}}\, \hat{\alpha}$, leads to[26]

$$P(\hat{\alpha},\chi_1 \oplus \chi_2;t) = \sum_{\hat{\beta}} \sum_{\hat{\gamma}} C^{\hat{\alpha}}_{\hat{\gamma},\hat{\beta}}\, P(\hat{\gamma},\chi_1;t) P(\hat{\beta},\chi_2;t). \tag{13}$$

Equations (8) and (13) demonstrate that the Poincaré series for reducible representations α and χ can always be expressed in terms of the series of their irreducible components $\hat{\alpha}$ and $\hat{\chi}$. Therefore, in the remainder of this paper we will consider only irreducible representations and corresponding $P(\hat{\alpha},\hat{\chi};t)$.

Starting from Eq. (9), it is easy to derive the following identity[27]:

$$P(\hat{\alpha},\hat{\chi};t) = (-t)^{\dim \hat{\chi}}\, P(\hat{\alpha} \det \hat{\chi},\hat{\chi}^*;\mathrm{t}^{-1}). \tag{14}$$

This, via Eq. (3) and

$$D(\hat{\chi}^*;t^{-1}) = D(\hat{\chi};t^{-1}) = (-t)^{-\dim \hat{\chi}} t^{-r(\hat{\chi})} D(\hat{\chi};t), \tag{15}$$

leads to

$$N(\hat{\alpha},\hat{\chi};t) = t^{r(\hat{\chi})} N(\hat{\alpha} \det \hat{\chi},\hat{\chi}^*;t^{-1}), \tag{16}$$

where $r(\hat{\chi}) = \Sigma_{i=1}^{\dim \hat{\chi}} [d_i(\hat{\chi}) - 1]$ (when the image of G under $\hat{\chi}$ is a reflection group, r equals the number of reflections). Consequently, the degree of $N(\hat{\alpha},\hat{\chi};t)$ cannot exceed $r(\hat{\chi})$. Furthermore, when $\hat{\chi} \sim \hat{\chi}^*$ and $\hat{\alpha} \det \hat{\chi} \sim \hat{\alpha}$, which is often the case, or when $\hat{\alpha} \det \hat{\chi} \sim \hat{\alpha}^*$, Eq. (16) implies that $N(\hat{\alpha},\hat{\chi};t)$ is a polynomial symmetric around the power $\frac{1}{2}r(\hat{\chi})$. These two remarks, which also hold for reducible α and χ, completely answer the first two questions raised at the end of Sec. I.

To proceed with other simple results, let us denote by $\hat{\chi}(G)$ the image of G under $\hat{\chi}$,

$$\hat{\chi}(G) = \operatorname{Im}_{\hat{\chi}}(G). \tag{17}$$

That is, $\hat{\chi}(G)$ is the group of matrices representing G under $\hat{\chi}$. Therefore, in deriving results pertinent to the G-action on V the only memory of G is through $\hat{\chi}(G)$, which is isomorphic to the quotient group $G/\operatorname{Ker}_G(\hat{\chi})$ [$\operatorname{Ker}_G(\hat{\chi})$ is the kernel of $\hat{\chi}$, i.e., it is the largest subgroup of G such that $\operatorname{Im}_{\hat{\chi}}(\operatorname{Ker}_G \hat{\chi}) = 1$]. In particular, we have the following.

Lemma 2.1: $\mathbb{C}[V]$ can carry only these representations $\hat{\alpha}$ of G which are also representations of $\hat{\chi}(G)$ such that $\operatorname{Ker}_G(\hat{\alpha}) \geqslant \operatorname{Ker}_G(\hat{\chi})$.

An immediate consequence of this lemma is the following corollary.

Corollary 2.1: If $P(\hat{\alpha},\hat{\chi};t) \neq 0$ then $\operatorname{Ker}_G \hat{\alpha} \geqslant \operatorname{Ker}_G(\hat{\chi})$.

The same conclusion could have been reached by observing that a symmetrized power of an identity matrix is another identity matrix. This line of reasoning leads us to consider the center of G, $\operatorname{Ctr}(G)$: it is the largest subgroup of G whose elements commute with all elements of G; it is an invariant subgroup of G, $\operatorname{Ctr}(G) \leqslant G$; it is also abelian. It is an immediate consequence of Schur's lemmas that elements of $\operatorname{Ctr}(G)$ will be represented by matrices proportional to the identity matrix in any irreducible representation $\hat{\chi}$. Hence, an observation that a symmetrized power of a scalar (= ma-

trix proportional to any identity matrix) is another scalar, results in some further and more refined results analogous to Corollary 2.1.

Since $\mathrm{Ctr}(G)$ is abelian and its representation under $\hat{\chi}$ is scalar (essentially one-dimensional), $\hat{\chi}[\mathrm{Ctr}(G)]$ must be isomorphic to a cyclic group $C_{c(\hat{\chi})}$, $c(\hat{\chi})$ being a divisor of $|\mathrm{Ctr}(G)|$ = order of Ctr (G) (see Refs. 28 and 29). Consequently, the mth symmetrized power of $\hat{\chi}[\mathrm{Ctr}(G)]$ is isomorphic to a cyclic group of order $c(\hat{\chi})/\gcd(c(\hat{\chi}),m)$,

$$\hat{\chi}[\mathrm{Ctr}(G)]^{[m]} \sim C_{c(\hat{\chi})/\gcd(c(\hat{\chi}),m)}, \tag{18}$$

where $\gcd(x,y,z,\ldots)$ denotes the greatest common divisor of x, y, z,... . This verifies the following lemmas.

Lemma 2.2: (a) $D(\hat{\chi};t)$ is a polynomial in $t^{c(\hat{\chi})}$, $D(\hat{\chi};t) = D'(\hat{\chi};t^{c(\hat{\chi})})$ [that is, $c(\hat{\chi})$ is a divisor of each $d_i(\hat{\chi})$, $i = 1,\ldots,\dim \hat{\chi}$, cf. Eq. (3) and Theorem 1.1.]; (b) if $P(\hat{\alpha},\hat{\chi};t) \neq 0$ then $c(\hat{\alpha})$ is divisor of $c(\hat{\chi})$; and (c) there exists an integer $n(\hat{\alpha})$, $0 \leqslant n(\hat{\alpha}) < c(\hat{\alpha})$, such that $N(\hat{\alpha},\hat{\chi};t)$ is a polynomial in $t^{c(\hat{\chi})}$ times $t^{n(\hat{\alpha})c(\hat{\chi})/c(\hat{\alpha})}$, $N(\hat{\alpha},\hat{\chi};t) = t^{n(\hat{\alpha})c(\hat{\chi})/c(\hat{\alpha})} N'(\hat{\alpha},\hat{\chi};t^{c(\hat{\chi})})$ [that is, each $\delta_j(\hat{\alpha},\hat{\chi})$, $j = 1,\ldots,l(\hat{\alpha},\hat{\chi})$, is equal to $n(\hat{\alpha})c(\hat{\chi})/c(\hat{\alpha})$ modulo $c(\hat{\chi})$, cf. Eq. (4) and Theorem 1.1].

An immediate corollary is the following.

Corollary 2.2: If $P(\hat{\alpha},\hat{\chi};t) \neq 0$ then $c(\hat{\alpha})$ divides $c(\hat{\chi})$ and

$$P(\hat{\alpha},\hat{\chi};t) = t^{n(\hat{\alpha})c(\hat{\chi})/c(\hat{\alpha})} \frac{N'(\hat{\alpha},\hat{\chi};t^{c(\hat{\chi})})}{D'(\hat{\chi};t^{c(\hat{\chi})})}, \quad 0 \leqslant n(\hat{\alpha}) < c(\hat{\alpha}). \tag{19}$$

It is clear at this point that one could make Corollary 2.2 [e.g., $n(\hat{\alpha})$]more precise. However, it is also clear that the main ingredient in deriving this corollary is the fact that $\mathrm{Ctr}(G)$ is represented by scalars in $\hat{\chi}$. Thus, we could obtain finer results by considering the subgroup of *all* scalars in $\hat{\chi}(G)$ which obviously includes $\hat{\chi}[\mathrm{Ctr}(G)]$. This is the line which we will pursue in the next section.

III. CENTERER AND p-PHASE

Following the motivation of the previous section let us focus on the group of all scalars in $\hat{\chi}(G)$. Since $\hat{\chi}$ is irreducible, this group is the center of $\hat{\chi}(G)$. Its inverse image under $\hat{\chi}$ we will call the *centerer* of $\hat{\chi}$ and we will denote it by $\mathrm{Zer}_G(\hat{\chi})$:

$$\mathrm{Zer}_G(\hat{\chi}) \equiv \mathrm{Im}_{\hat{\chi}}^{-1}\{\mathrm{Ctr}[\hat{\chi}(G)]\}. \tag{20}$$

That is, $\mathrm{Zer}_G(\hat{\chi})$ is the largest subgroup of G such that its elements are represented under $\hat{\chi}$ by scalar matrices.

It is straightforward to prove the following properties of $\mathrm{Zer}_G(\hat{\chi})$:

$$\mathrm{Zer}_G(\hat{\chi}) \trianglerighteq \mathrm{Ker}_G(\hat{\chi}); \tag{21}$$

$$\mathrm{Zer}_G(\hat{\chi}) \trianglerighteq \mathrm{Ctr}(G); \tag{22}$$

$$\mathrm{Zer}_G(\hat{\chi}) \trianglelefteq G. \tag{23}$$

Furthermore, it can be seen, just as in the case of $\mathrm{Ker}_G(\hat{\chi})$, that the definition is "good," i.e., $\mathrm{Zer}_G(\hat{\chi})$ is independent of a particular realization of $\hat{\chi}$ within its equivalence class. In fact, $\mathrm{Zer}_G(\hat{\chi})$ can be easily determined directly from the character tables:

$$\mathrm{Zer}_G(\hat{\chi}) = \{g: g \in G, |\mathrm{tr}[\hat{\chi}(g)]| = \dim \hat{\chi}\}. \tag{24}$$

Therefore, we see that $\mathrm{Zer}_G(\hat{\chi})$ is a natural next step from $\mathrm{Ker}_G(\hat{\chi})$.[30,31]

Since Ctr $[\hat{\chi}(G)]$ is an abelian, scalar matrix group it must be a cyclic group

$$\mathrm{Ctr}[\hat{\chi}(G)] \sim C_{p(\hat{\chi})} \tag{25}$$

of order (period)

$$p(\hat{\chi}) = |\mathrm{Ctr}[\hat{\chi}(G)]| = |\mathrm{Zer}_G(\hat{\chi})/\mathrm{Ker}_G(\hat{\chi})|. \tag{26}$$

It can be written as

$$\mathrm{Ctr}[\hat{\chi}(G)] = \{z(\hat{\chi})^j\}_{j=1}^{p(\hat{\chi})}, \quad z(\hat{\chi}), = e^{2\pi i/p(\hat{\chi})}. \tag{27}$$

Therefore, following a similar argument that led to Corollaries 2.1. and 2.2. we find the following lemma.

Lemma 3.1: If $P(\hat{\alpha},\hat{\chi};t) \neq 0$ then $\mathrm{Ker}_G(\hat{\alpha}) \geqslant \mathrm{Ker}_G(\hat{\chi})$ *and* $\mathrm{Zer}_G(\hat{\alpha}) \geqslant \mathrm{Zer}_G(\hat{\chi})$.

Let us now consider $g_1, g_2 \in \mathrm{Im}_{\hat{\chi}}^{-1}[z(\hat{\chi})]$ and let us assume that the conditions of Lemma 3.1. are fulfilled. Then $\hat{\alpha}(g_1)$ and $\hat{\alpha}(g_2)$ are also scalars. Furthermore, for every integer n, $g_1^n g_2^{p(\hat{\chi})-n} \in \mathrm{Ker}_G(\hat{\chi}) \leqslant \mathrm{Ker}_G(\hat{\alpha})$, implies

$$\hat{\alpha}(g_1)^n \hat{\alpha}(g_2)^{p(\hat{\chi})-n} = 1. \tag{28}$$

In particular, taking $n = 0$ and 1, one finds $\hat{\alpha}(g_1) = \hat{\alpha}(g_2)$ and $\hat{\alpha}(g_1)^{p(\hat{\chi})} = 1$. Therefore, there exists an integer $n(\hat{\alpha},\hat{\chi})$, $0 \leqslant n(\hat{\alpha},\hat{\chi}) < p(\hat{\chi})$, such that

$$\hat{\alpha}\{\mathrm{Im}_{\hat{\chi}}^{-1}[z(\hat{\chi})]\} = \{z(\hat{\chi})^{n(\hat{\alpha},\hat{\chi})}\} \tag{29}$$

and we say that $\hat{\alpha}$ has a definite $p(\hat{\chi})$-phase with respect to $\hat{\chi}$, namely, $n(\hat{\alpha},\hat{\chi})$. The phase can easily be determined from the character tables.[32]

We are now in the position to generalize Lemma 2.2.

Lemma 3.2: (a) $D(\hat{\chi};t)$ is a polynomial in $t^{p(\hat{\chi})}$, $D(\hat{\chi};t) \equiv \overline{D}(\hat{\chi};t^{p(\hat{\chi})})$ [that is, $p(\hat{\chi})$ is a divisor of each $d_i(\hat{\chi})$, $i = 1,\ldots,\dim \hat{\chi}$]; and (b) $\overline{N}(\hat{\alpha},\hat{\chi};t)$ is a product of $t^{n(\hat{\alpha},\hat{\chi})}$ and a polynomial in $t^{p(\hat{\chi})}$, $N(\hat{\alpha},\hat{\chi};t) \equiv t^{n(\hat{\alpha},\hat{\chi})}\overline{N}(\hat{\alpha},\hat{\chi};t^{p(\hat{\chi})})$ [that is, each $\delta j(\hat{\alpha},\hat{\chi})$, $j = 1,\ldots,l(\hat{\alpha},\hat{\chi})$, is equal to $n(\hat{\alpha},\hat{\chi})$ modulo $p(\hat{\chi})$].

Therefore, we have the corollary which generalizes Corollary 2.2.

Corollary 3.1: If $P(\hat{\alpha},\hat{\chi};t) \neq 0$ then there exists $n(\hat{\alpha},\hat{\chi})$, $0 \leqslant n(\hat{\alpha},\hat{\chi}) < p(\hat{\chi})$, such that

$$P(\hat{\alpha},\hat{\chi};t) = t^{n(\hat{\alpha},\hat{\chi})}[\overline{N}(\hat{\alpha},\hat{\chi};t^{p(\hat{\chi})})/\overline{D}(\hat{\chi};t^{p(\hat{\chi})})]. \tag{30}$$

It can be verified that Eq. (30) does not contradict Eq. (19) since $c(\hat{\chi})$ divides $p(\hat{\chi})$.

The main results of this paper are Lemma 3.1. and Corollary 3.1 which answer the last question of Sec. I. In the remainder of this section we will show how these results may be used to relate the Poincaré series $P(\hat{\alpha},\hat{\epsilon}\hat{\chi};t)$ to the Poincaré series for $P(\hat{\alpha}\hat{\epsilon}^{-q},\hat{\chi};t)$, $q = 1,\ldots,p(\hat{\epsilon})$, $\hat{\epsilon}$ being a linear (one-dimensional) character. The formula we seek to prove is

$$P(\hat{\alpha},\hat{\epsilon}\hat{\chi};t) = \sum_{q=1}^{p(\hat{\epsilon})} \mathscr{P}[q \bmod p(\hat{\epsilon})] P(\hat{\alpha}\hat{\epsilon}^{-q},\hat{\chi};t), \tag{31}$$

where the projector $\mathscr{P}[q \bmod p(\hat{\epsilon})]$ picks the powers $q \bmod p(\hat{\epsilon})$ out of a power series. The sum need extend only over these q for which $\mathrm{Ker}_G(\hat{\alpha}\hat{\epsilon}^{-q}) \geqslant \mathrm{Ker}_G(\hat{\chi})$ and $\mathrm{Zer}_G(\hat{\alpha}\hat{\epsilon}^{-q}) \geqslant \mathrm{Zer}_G(\hat{\chi})$.

The first step in deriving Eq. (31) is

$$P(\hat{\alpha},\hat{\epsilon}\hat{\chi};t) = \sum_{\hat{\beta}} \langle \mathrm{tr}[\hat{\beta}(g)] P(\hat{\alpha}\times\hat{\beta},\hat{\chi};\hat{\epsilon}(g)t)\rangle, \tag{32}$$

which follows from Eqs. (9) and (12) and the fact that $\hat{\epsilon}(g)$ is a scalar (complex number). On the other hand, using the original definition [Eq. (1)] one easily verifies that the terms which survive in Eq. (32) are only those for which $\hat{\beta} = \hat{\epsilon}^{-q}$,

$q = 1,2,\ldots,p(\hat{\epsilon})$. Thus,

$$P(\hat{\alpha},\hat{\epsilon}\hat{\chi};t) = \sum_{q=1}^{p(\hat{\epsilon})} \langle \hat{\epsilon}^{-q}(g) P(\hat{\alpha}\hat{\epsilon}^{-q},\hat{\chi};\hat{\epsilon}(g)t)\rangle. \tag{33}$$

The next step is to observe that

$$\langle F[\hat{\epsilon}(g)]\rangle = \frac{1}{p(\hat{\epsilon})} \sum_{a=1}^{p(\hat{\epsilon})} F[e^{2\pi i a/p(\hat{\epsilon})}]. \tag{34}$$

Furthermore, it follows from Lemma 3.1 that $P(\hat{\alpha}\hat{\epsilon}^{-q},\hat{\chi};t)$ is identically zero unless $\mathrm{Ker}_G(\hat{\alpha}\hat{\epsilon}^{-q}) \geqslant \mathrm{Ker}_G(\hat{\chi})$ and $\mathrm{Zer}_G(\hat{\alpha}\hat{\epsilon}^{-q}) \geqslant \mathrm{Zer}_G(\hat{\chi})$. Therefore, by applying Eq. (34) to Eq. (33), we arrive at the result [Eq. (31)].

In order to illustrate the relationship [Eq. (31)] we consider the octahedral group O. The Poincaré series for this group have been calculated in Ref. 17 whose notation we adopt. Let us take $\hat{\chi} = \Gamma_5$ and $\hat{\epsilon} = \Gamma_2$. Using the character tables we find $\Gamma_2\Gamma_5 = \Gamma_4$, $p(\Gamma_2) = 2$ and $\Gamma_2^{-1} = \Gamma_2$. Thus, Eq. (31) reduces to

$$P(\hat{\alpha},\Gamma_4;t) = \mathscr{P}[0 \bmod 2] P(\hat{\alpha},\Gamma_5;t) + \mathscr{P}[1 \bmod 2] P(\hat{\alpha}\Gamma_2,\Gamma_5;t). \tag{35}$$

Let us first take $\hat{\alpha} = \Gamma_1$. From Ref. 17 we find $P(\Gamma_1,\Gamma_5;t) = 1/(1-t^2)(1-t^3)(1-t^4)$ and $P(\Gamma_2,\Gamma_5;t) = t^6/(1-t^2)(1-t^3)(1-t^4)$ so that Eq. (35) leads to $P(\Gamma_1,\Gamma_4;t) = (1+t^9)/(1-t^2)(1-t^4)(1-t^6)$ as is indeed the case. If we now take $\hat{\alpha} = \Gamma_3$ and observe that $\Gamma_3\Gamma_2 = \Gamma_3$ we find using Eq. (35) $P(\Gamma_3,\Gamma_4;t) = P(\Gamma_3,\Gamma_5;t)$. The right-hand side is, cf. Ref. 17, $(t^2+t^4)/(1-t^2)(1-t^3)(1-t^4)$ which needs to be written with the denominator of $P(\Gamma_1,\Gamma_4;t)$ to get $P(\Gamma_3,\Gamma_4;t)$ carrying the information on Γ_3 covariants of Γ_4: $P(\Gamma_3,\Gamma_4;t) = (t^2+t^4+t^5+t^7)/(1-t^2)(1-t^4)(1-t^6)$. One can similarly determine all $P(\hat{\alpha},\Gamma_4;t)$ using Eq. (35). In all the cases $N(\hat{\alpha},\Gamma_4;t)$ is symmetric around the power $\frac{9}{2}$ which, as explained in previous section, is due to the fact that $\Gamma_4^* \sim \Gamma_4$, $\det \Gamma_4 = \Gamma^1 = 1$ and $r(\Gamma_4) = (2-1) + (4-1) + (6-1) = 9$.

IV. CONCLUSIONS

We showed in this brief paper how various characteristics of Poincaré series can be understood on the basis of structure of irreducible images of a group. In particular, we showed that an important role is played by the center of an image and, consequently, by its inverse image which we called the centerer. For example, we proved that all $\hat{\alpha}$-covariants which can be constructed from symmetrized powers of $\hat{\chi}$ must have a definite $p(\hat{\chi})$-phase, i.e., a definite degree modulo $p(\hat{\chi})$. Furthermore, we exemplified a use of the results of this paper to derive a formula for relating the Poincaré series $P(\hat{\alpha},\hat{\epsilon}\hat{\chi};t)$ with the series $P(\hat{\alpha}\hat{\epsilon}^{-q},\hat{\chi};t)$, $q = 1,\ldots,p(\hat{\epsilon})$, whenever $\hat{\epsilon}$ is a linear character.

ACKNOWLEDGMENTS

The author acknowledges the hospitality of the Institut des Hautes Etudes Scientifiques and an Alexander von Humboldt research fellowship during the initial stages of this work. He is also grateful to Prof. R. T. Sharp for several stimulating and illuminating discussions. He also thanks Professor G. W. Schwartz for pointing out some difficulties in extending the results of this paper to infinite, compact groups (see, for example, Ref. 27).

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[24] Even such a simple relation as $P(\alpha,\chi;t) = P(\alpha^*,\chi^*;t)$ is often not stated. [Here and throughout the paper * denotes complex conjugation and t is assumed real.]

[25] Note that our $P(\alpha_1 \otimes \alpha_2, \chi;t)$ is different from $P(\alpha_1 \otimes \alpha_2,\chi;t_1t_2) = P(\alpha_1,\chi;t_1)P(\alpha_2,\chi;t_2)$ whose coefficient of $t_1^{m_1} t_2^{m_2}$ is the number of linearly independent $\alpha_1 \oplus \alpha_2$ covariants such that α_1 is of the power m_1 and α_2 is of the power m_2 in χ (cf. Ref. 17).

[26] Reference 17 defines $P(\hat{\alpha},\chi_1 \oplus \chi_2;t_1,t_2)$ whose coefficient by $t_1^{m_1} t_2^{m_2}$ is the number of linearly independent $\hat{\alpha}$-covariants of degrees m_1 and m_2 in χ_1 and χ_2, respectively. Clearly $P(\hat{\alpha},\chi_1 \oplus \chi_2;t) = P(\hat{\alpha}\chi_1 \oplus \chi_2;t,t)$ and our Eq. (13) is a special case of an equation given in Ref. 17.

[27] This may fail for an infinite group for which $P(\hat{\alpha},\hat{\chi};t^{-1}) \neq \langle \mathrm{tr}\, \hat{\alpha}(g)^* \det[1 - t^{-1}\hat{\chi}(g)]^{-1}\rangle 1$ when t is sufficiently small so that Eq. (9) holds. For example, for O(2) one has $P(m,1;t) = t^m/(1-t^2)$ so that $P(m,1;t^{-1}) = t^{-m}/(1-t^{-2})$ while the use of Eq. (9) gives $-t^m/(1-t^2)$ whenever $|t| < 1$.

[28] Although some of the results will be generalizable to infinite, compact groups we again emphasize that all the groups we consider are finite.

[29] Since $\mathrm{Ctr}(G)$ is abelian and finite it can be decomposed into a direct product of cyclic groups; $\mathrm{Ctr}(G) = C_{n_1} \times C_{n_2} \times \cdots$, with $|\mathrm{Ctr}(G)| = n_1 n_2 \cdots$. Therefore, a one-dimensional (scalar) representation of $\mathrm{Ctr}(G)$ must be isomorphic to a cyclic group of order $c(\hat{\chi})$ which is a divisor of $\mathrm{lcm}(n_1,n_2,\ldots)$ = the least common multiple of $n_1,n_2,\ldots$.

[30] Since G is finite, one easily shows that $\mathrm{Ctr}(G) = \cap_{\hat{\alpha}} \mathrm{Zer}_G(\hat{\alpha})$.

[31] For example, $\mathrm{Ctr}\, SU(N) = C_N$. In its adjoint representation $\mathrm{Zer}_{SU(N)} = C_N$, $\mathrm{Ker}_{SU(N)} = C_1$.

[32] Consider, for example $\hat{\chi} = E$ for D_{3h} [Table 4-17 in M. Hamermesh, *Group Theory and its Application to Physical Problems* (Addison–Wesley, Reading, MA, 1962)]. $\mathrm{Ctr}(D_{3h}) = C_s \sim C_2$, $\mathrm{Zer}_{D_{3h}}(E'') = C_s \mathrm{Ker}_{D_{3h}}(E'') = C_1$. Now take $\hat{\alpha} = E'$ for which $\mathrm{Zer}_{D_{3h}}(E') = \mathrm{Ker}_{D_{3h}}(E') = C_s$ so the conditions of Lemma 3.1. are fulfilled. Then $n(E',E'') = 0$. Similarly, $n(A_2'',E'') = 1$, etc.

[33] One can project out from any power series $F(t)$ the part which contains only powers n mod p using the projector $\mathscr{P}[n \bmod p]$ defined by $\mathscr{P}[n \bmod p] F(t) = (1/p) \sum_{j=1}^{p} e^{-2\pi i j n/p} F(e^{2\pi i j/p} t)$.

Lie groups and Lie algebras with generalized supersymmetric parameters

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(Received 30 June 1983; accepted for publication 25 May 1984)

Matrices with σ-symmetric parameters (the most general extension of supersymmetric parameters) are investigated. The superdeterminants of such matrices are defined. Lie groups consisting of these matrices and their Lie algebras are studied.

PACS numbers: 02.20. + b, 11.30.Pb

I. INTRODUCTION

Lie superalgebras and Lie supergroups have been utilized extensively in physics.[1] In those theories, Grassmann algebras play an important role. In fact, the theory of supermanifolds and supergroups are formulated on the basis of Grassman algebras.[2–6] They have been also used in describing Fermi systems.[7] Ohnuki and Kamefuchi[8–11] have introduced generalized Grassmann numbers and generalized Bose numbers to describe para-Fermi and para-Bose systems. They also considered the groups parametrized in these numbers.

On the other hand, Rittenberg and Wyler[12,13] tried to go beyond supersymmetry and introduced color algebras and color superalgebras. Their concept was beautifully formulated as generalized Lie algebras by Scheunert[14] (see also Agrawala[15]). The supersymmetry in his sense is considered to be the most general with respect to the concept of commutativity. We call the (associative) algebras with this generalized supersymmetry the σ-commutative algebras and adopt them as a basis of our theory. It is interesting that a σ-commutative algebra has appeared in a quark confinement model[16] (see example 2.3).

In the present work we shall develop the theory of matrices whose entries are elements of a σ-commutative algebra (matrices with σ-symmetric parameters) and study the algebras and the groups consisting of these matrices.

The paper is organized as follows. In Sec. II, we give some fundamental concepts which are basically formulated by Scheunert. In Sec. III, we define the (super) determinant of a matrix with σ-symmetric parameters and give its basic properties. Our definition is a generalization of Leites,[17] Ohnuki and Kamefuchi,[8] and Rittenberg and Wyler.[12] In Sec. IV, we study the groups of matrices with σ-symmetric parameters and their Lie algebras. In Sec. V, we give a natural way to associate a superobject with a σ-symmetric one.

We hope that this work will be a first step to the generalization of the theory of supersymmetry.

We express our thanks to the referee who helped us to correct some errors contained in the original version of this paper.

II. σ-SYMMETRY (GENERALIZED SUPERSYMMETRY)

Let k be a field whose characteristic is not equal to 2 and let G be an abelian (additive) group.

Definition 2.1: A mapping $\sigma: G \times G \to k$ is a *sign* (*commutation factor* in terms of Sheunert[14]) of G, if σ satisfies

$$\text{(i)}\quad \sigma(\alpha+\beta,\gamma)=\sigma(\alpha,\gamma)\sigma(\beta,\gamma),$$
$$\text{(ii)}\quad \sigma(\alpha,\beta)\sigma(\beta,\alpha)=1, \tag{2.1}$$

for any $\alpha, \beta, \gamma \in G$. The pair (G,σ) is called a *signed group*.

A base field k and a signed group (G,σ) are fixed throughout this paper. It is easy to see that $\sigma(\alpha,\alpha)$ is either 1 or -1 for any $\alpha \in G$. An element α of G is called *even* (resp. *odd*), if $\sigma(\alpha,\alpha)=1$ (resp. -1). Here G_0 (resp. G_1) denotes the set of all even (resp. odd) elements of G. When $G_1=\emptyset$, G is called *even*. Here G_0 is a subgroup of G of index at most 2 and we have $G=G_0 \cup G_1$ (disjoint union).

A G-graded (associative) algebra $A=\oplus_{\alpha\in G}A_\alpha$ over k is called *σ-commutative* or *σ-symmetric*, if

$$ab=\sigma(\alpha,\beta)ba$$

holds for any $\alpha, \beta \in G$ and $a \in A_\alpha$, $b \in A_\beta$.

Let $V=\oplus_{\alpha\in G}V_\alpha$ be a G-graded vector space over k. Let $T(V)$ be the tensor algebra of V over k and I be the ideal of $T(V)$ generated by the elements of the form

$$x \otimes y - \sigma(\alpha,\beta)\cdot y \otimes x,$$

where $\alpha, \beta \in G$ and $x \in V_\alpha$, $y \in V_\beta$. The quotient algebra $\tilde{U}(V)=T(V)/I$ is σ-commutative and is called the *σ-symmetric algebra* of V over k.

Let A and B be two G-graded algebras over k. The G-graded vector space

$$A \otimes_k B=\oplus_{\alpha\in G}\left(\oplus_{\beta+\gamma=\alpha}(A_\beta \otimes_\beta B_\gamma)\right)$$

is a G-graded algebra, if we define the multiplication by

$$(a\otimes b)\cdot(c\otimes d)=\sigma(\beta,\gamma)(ac\otimes bd)$$

for $\beta, \gamma \in G$ and $a \in A$, $b \in B_\beta$, $c \in A_\gamma$, $d \in B$. The algebra $A \otimes_k B$ is called the *graded tensor product* of A and B over k. If A and B are σ-commutative, so is $A \otimes_k B$.

Example 2.2: Let $G=Z_2 \oplus \cdots \oplus Z_2$ be the direct sum of l copies of $Z_2=Z/2Z$. Let $i=(0,\ldots,0,1,0,\ldots,0)\in G$ be the ith unit vector. If we define $\sigma(i,j)$ to be 1 or -1 for all i, $j=1,\ldots,l$ with $i \leqslant j$, σ can be uniquely extended to a sign of G. Let $V=\oplus V_i$ be a G-graded vector space over the real number field $\mathbb{R}$ such that V_i is a one-dimensional vector space over $\mathbb{R}$ with a generator of grade i. The σ-symmetric algebra $\tilde{U}(V)$ of V over $\mathbb{R}$ is the generalized number system of Ohnuki–Kamefuchi.[8,9]

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Example 2.3: Let n be a positive integer. Let $G = Z_n \oplus \cdots \oplus Z_n$ be a direct sum of $2l$ copies of $Z_n = Z/nZ$. Define a sign of G by

$$\sigma(i,j) = \begin{cases} \exp(2\pi\sqrt{-1}/n), & \text{if } j-i=l, \\ 1, & \text{otherwise,} \end{cases}$$

for $i,j = 1,\ldots,2l$ with $i \leqslant j$, where i is the same as in Example 2.2. A G-graded vector space V is also defined in the same way as in Example 2.2. Then the σ-symmetric algebra $\tilde{U}(V)$ of V is the operator algebra appeared in the theory of quark confinement in SU(n) gauge theory by 't Hooft.[16]

Example 2.4: The quaternion field $\mathbb{H}$ is considered to be a σ-commutative algebra over $\mathbb{R}$ as follows. Let $\{1,i,j,k\}$ be the usual basis of $\mathbb{H}$. Let $G = Z_2 \oplus Z_2$ and define a sign σ of G by $\sigma((l,m),(n,p)) = (-1)^{mn-lp}$ for $l, m, n, p \in Z_2$. The gradation of $\mathbb{H}$ is given by $g(1) = (0,0)$, $g(i) = (1,0)$, $g(j) = (0,1)$ and $g(k) = (1,1)$.

Definition 2.5: Let F be a σ-commutative algebra over k. A G-graded algebra $L = \oplus_{\alpha\in G} L_\alpha$ over k with bilinear operation $\langle .,. \rangle$ is called a *G-graded Lie σ-algebra over F*, if the following hold: (i) L is a G-graded left F-module, that is, $aX \in L_{\alpha+\beta}$ for any $\alpha, \beta \in G$ and $a \in F_\alpha$, $X \in L_\beta$;

(ii) $\langle aX, Y \rangle = a\langle X, Y \rangle$, for any $a \in F$ and $X, Y \in L$; (2.2)

(iii) $\langle X, Y \rangle + \sigma(\alpha,\beta)\langle Y, X \rangle = 0$, for any $\alpha, \beta \in G$ and $X \in L_\alpha$, $Y \in L_\beta$; (2.3)

(iv) $\sigma(\gamma,\alpha)\langle X, \langle Y, Z \rangle \rangle + \sigma(\beta,\gamma)\langle Z, \langle X, Y \rangle \rangle + \sigma(\alpha,\beta)\langle Y, \langle Z, X \rangle \rangle = 0$,

for any $\alpha, \beta, \gamma \in G$ and $X \in L_\alpha$, $Y \in L_\beta$, $Z \in L_\gamma$.

If the characteristic of k is 3, we need to add the identity $\langle X, \langle X, X \rangle \rangle = 0$. Our definition above is a combination of Sheunert's generalized Lie algebra[14] and Rogers' graded Lie module.[6] Let $\alpha, \beta \in G$ and $a \in F_\beta$, $X \in L_\alpha$, $Y \in L$. Then by (2.1)–(2.3) we easily have

$$\langle X, aY \rangle = \sigma(\alpha,\beta) a \langle X, Y \rangle.$$

In this sense the operation $\langle .,. \rangle$ is F-bilinear.

The identity element of G is always denoted by 0. For a G-graded Lie σ-algebra L over F, the component L_0 of grade 0 of L is an (ordinary) Lie algebra over k and called the *Lie part* of L.

Definition 2.6: A mapping $\phi: G \times G \to k \setminus \{0\}$ is called a *factor system* (*multiplier* in terms of Scheunert[14]) on G, if it satisfies

(i) $\phi(\alpha, \beta+\gamma)\phi(\beta,\gamma) = \phi(\alpha,\beta)\phi(\alpha+\beta,\gamma)$, for any $\alpha, \beta, \gamma \in G$, (2.4)

(ii) $\phi(0,0) = 1$.

It follows from (2.4) that

$$\phi(\alpha,0) = \phi(0,\alpha) = 1, \tag{2.5}$$

$$\phi(\alpha,-\alpha) = \phi(-\alpha,\alpha) = \phi(\alpha,\beta)\phi(-\alpha,\alpha+\beta), \tag{2.6}$$

for any $\alpha, \beta \in G$.

As is well-known, if a factor system ϕ on G is given, we can construct a G-graded σ-commutative algebra $C = \oplus_{\alpha\in G} C_\alpha$ over k, called the *crossed product* of k and G as follows: C_α is a one dimensional vector space over k with a generator u_α of grade α. The multiplication in C is given by

$$u_\alpha \cdot u_\beta = \phi(\alpha,\beta) u_{\alpha+\beta},$$

for $\alpha, \beta \in G$. By (2.5), u_0 is an identity element of C. The following is due to Scheunert.[14]

Proposition 2.7: Let (G,σ) be an even signed group and assume that G is finitely generated. Then there is a factor system ϕ on G such that

$$\sigma(\alpha,\beta) = \phi(\alpha,\beta)/\phi(\beta,\alpha),$$

for $\alpha, \beta \in G$. Moreover, if $|\sigma(\alpha,\beta)| = 1$ for all $\alpha, \beta \in G$, we can choose ϕ so that $|\phi(\alpha,\beta)| = 1$ for all $\alpha, \beta \in G$.

For the later use we extend the signed group (G,σ) as follows. Let

$$\bar{G} = G \oplus Z_2 \tag{2.7}$$

and define a sign $\bar{\sigma}$ of $\bar{G}$ by

$$\bar{\sigma}((\alpha,m),(\beta,n)) = \sigma(\alpha,\beta)(-1)^{mn}, \tag{2.8}$$

for $\alpha, \beta \in G$ and $m, n \in Z_2$.

III. SUPERDETERMINANT

In this section $F = \oplus_{\alpha\in G} F_\alpha$ is a G-graded σ-commutative algebra over k wih identity element 1.

A finite set I is called a *G-set*, if it is linearly ordered and a grade $g(i) \in G$ is assigned to every element i of I. Let I be a G-set. Another G-set $-I = \{-i; i \in I\}$ is defined in such a way that $-i < -j$ if $j < i$ and $g(-i) = -g(i)$ for $i, j \in I$. A subset I' of I is a G set with the order and the gradation of I restricted to I'. Here $|I|$ denotes the cardinality of I. We also define $g(I) = \Sigma_{i\in I} g(i)$.

Definition 3.1: Let I and J be G-sets and let $\alpha \in G$. *A $|I| \times |J|$ matrix $M = (M^i_j)$ over F is called an $I \times J$ matrix over F of grade α*, if

$$M^i_j \in F_{g(i)-g(j)+\alpha},$$

for every $i \in I$ and $j \in J$. An $I \times J$ matrix over F of grade 0 is most important and is called simply and *$I \times J$ matrix over F*.

Let I, J, and K be G-sets and let $\alpha, \beta \in G$. Let M be an $I \times J$ matrix over F of grade α and N a $J \times K$ matrix over F of grade β. Then the product MN is an $I \times J$ matrix over F of grade $\alpha + \beta$. For an element f of F of grade $\gamma \in G$, we define the scalar multiplications fM and Mf by

$$(fM)^i_j = \sigma(g(i),\gamma) f M^i_j \quad \text{and} \quad (Mf)^i_j = \sigma(g(j),\gamma) M^i_j f. \tag{3.1}$$

Then the natural associativity properties are fulfilled and

$$fM = \sigma(\gamma,\alpha) Mf$$

holds. Therefore we have the following.

Proposition 3.2: The algebra of all $|I| \times |J|$ matrices over F is a G-graded algebra over F, in which the $I \times I$ matrices of grade $\alpha \in G$ form the homogeneous component of grade α. It is a G-graded Lie σ-algebra over F with operation $\langle \cdot,\cdot \rangle$ defined by

$$\langle M, N \rangle = MN - \sigma(\alpha,\beta) NM$$

for $I \times I$ matrices M and N of grade α and β, respectively.

The G-graded Lie σ-algebra in Proposition 3.2 is called the *general linear Lie σ-algebra of degree I over F* and is denoted by $\mathfrak{gl}(I,F)$. The Lie part of $\mathfrak{gl}(I,F)$, that is, the Lie algebra of $I \times I$ matrices over F (of grade 0), is called the *general linear Lie algebra of degree I with parameters in F*,

and is denoted by $\mathrm{gl}(I,F)$. Note that there is the canonical isomorphism of $F\otimes_k \mathrm{gl}(I,k)$ onto $\mathrm{gl}(I,F)$ which sends $f\otimes M$ to fM.

A G-set I is called *even* (resp. *odd*), if the grade of every element of I is even (resp. odd). If I is either even or odd, I is called *unmixed*. An $I\times J$ matrix over F (of grade 0) is called *even* (resp. *odd, unmixed*), if $I\cup J$ is also.

We shall define the determinant first for odd matrices, next for even matrices, and finally we shall unify them.

Let I and J be G-sets with $|I| = |J|$. Assume that J is odd. Let x^j $(j\in J)$ be indeterminates of grade $g(j)$ and let $k[x] = k[x^j; j\in J]$ be the σ-symmetric algebra generated by x^j $(j\in J)$ over k (the σ-symmetric algebra of the vector space with basis $\{x^j; j\in J\}$ over k).

Definition 3.3: The *determinant* $\det M$ of an $I\times J$ matrix M with J odd is defined by the equation in $F[x] = F\otimes_k k[x]$,

$$\sum_{\pi}\prod_{i\in I} M^{i}_{\pi(i)}x^{\pi(i)} = \det M\cdot\prod_{j\in J}x^j,$$

where π ranges over all the bijections of I to J, and $\Pi_{j\in I}$ and $\Pi_{j\in J}$ mean the ordered product, for example, $\Pi_{j\in J}x^j = x^{j_1}x^{j_2}\cdots x^{j_n}$ if $J = \{j_1, j_2,\ldots, j_n\}$ and $j_1 < j_2 < \cdots < j_n$.

Next, let J be an even G-set. Let $(\bar{G},\bar{\sigma})$ be the signed group defined by (2.7) and (2.8). Let y^j $(j\in J)$ be indeterminates of odd grade $(g(j),1)\in\bar{G}$ and let $k[y] = k[y^j; j\in J]$ be the σ-symmetric algebra generated by y^j $(j\in J)$ over k.

Definition 3.4: The *determinant* $\det M$ of an $I\times I$ matrix M with J even is defined by the equation in $F[y] = F\otimes_k k[y]$,

$$\sum_{\pi}\prod_{i\in I} M^{i}_{\pi(i)}y^{\pi(i)} = \det M\cdot\prod_{j\in J}y^j,$$

where π, $\Pi_{i\in I}$, $\Pi_{j\in J}$ are the same as in Definition 3.3.

Our determinants have similar properties to those that the ordinary determinants have.

Proposition 3.5: Let I and J be G-sets such that $|I| = |J|$ and J is unmixed. Let M be an $I\times J$ matrix over F Then we have the following.

(i) $\det M\in F_{g(I)-g(J)}$.

(ii) Let $i_0\in I$ and let L and N be $I\times J$ matrices such that $M^{i_0}_j = L^{i_0}_j + N^{i_0}_j$ for every $j\in J$ and $M^{i}_j = L^{i}_j = N^{i}_j$ for every $j\in J$ and $i\in I$ with $i\neq i_0$. Then $\det M = \det L + \det N$.

(iii) Let i_1 and i_2 be different elements of I such that $g(i_1) = g(i_2)$. Assume that $I\cup J$ is unmixed. If $M^{i_1}_j = M^{i_2}_j$ for every $j\in J$, then $\det M = 0$.

Proof: Since (i) and (ii) are clear by the definitions of determinants, we only prove (iii). Assume $I\cup J$ is odd and $i_1 < i_2$. Let π be a bijection of I to J. Let π' be the bijection of I to J determined by $\pi'(i_1) = \pi(i_2)$, $\pi'(i_2) = \pi(i_1)$ and $\pi'(i) = \pi(i)$ for $i\neq i_1, i_2$. Then

$$\det M\cdot\prod_{j\in J}x^j = \sum_{\pi}\prod_{i\in I} M^{i}_{\pi(i)}x^{\pi(i)}$$

contains a pair of terms

$$\prod_{i\in I} M^{i}_{\pi(i)}x^{\pi(i)} = \cdots M^{i_1}_k x^k\cdots M^{i_2}_l x^l\cdots \tag{3.2}$$

and

$$\prod_{i\in I} M^{i}_{\pi'(i)}x^{\pi'(i)} = \cdots M^{i_1}_l x^l\cdots M^{i_2}_k x^k\cdots . \tag{3.3}$$

We have $g(M^{i_1}_k x^k) = g(i_1) - g(k) + g(k) = g(i_1)$ and $g(M^{i_2}_l x^l) = g(i_2)$. Hence, if we interchange $M^{i_1}_k x^k$ and $M^{i_2}_l x^l$ in (3.2), $\sigma(g(i_1), g(i_2)) = -1$ comes out. Therefore the terms (3.2) and (3.3) cancel, because $M^{i_1}_k = M^{i_2}_k$ and $M^{i_1}_l = M^{i_2}_l$. It follows that $\det M = 0$. The case when $I\cup J$ is even is similar.

Theorem 3.6: Let I, J, and K be G-sets such that $|I| = |J| = |K|$ and $J\cup K$ is unmixed. Let M be an $I\times J$ matrix and N a $J\times K$ matrix. Then we have

$$\det MN = \det M\cdot\det N. \tag{3.4}$$

Proof: Let us assume that $I\cup K$ is odd (the even case is similar). We have

$$\det M\cdot\det N\cdot\prod_{k\in K}x^k = \det M\cdot\sum_{\pi}\prod_{j\in J}N^{j}_{\pi(j)}x^{\pi(j)}$$

$$= \sum_{\pi}\det M\cdot\prod_{j\in J}N^{j}_{\pi(j)}x^{\pi(j)}.$$

Since $g(N^{j}_{\pi(j)}x^{\pi(j)}) = g(j)$, the last term is equal to

$$\sum_{\pi}\sum_{\mu}\prod_{i\in I} M^{i}_{\mu(i)}N^{\mu(i)}_{\pi\mu(i)}x^{\pi\mu(i)} = \sum_{\nu}\sum_{\mu}\prod_{i\in I} \times M^{i}_{\mu(i)}N^{\mu(i)}_{\nu(i)}x^{\nu(i)}, \tag{3.5}$$

where π (resp. μ, ν) ranges over all the bijections of J (resp. I,I) to K (resp. J,K). On the other hand

$$\det MN\cdot\prod_{k\in K}x^k = \sum_{\nu}\prod_{i\in I}\left(\sum_{j\in J}M^{i}_{j}N^{j}_{\nu(i)}\right)x^{\nu(i)}$$

$$= \sum_{\nu}\sum_{\bar{\mu}}\prod_{i\in I} M^{i}_{\bar{\mu}(i)}N^{\bar{\mu}(i)}_{\nu(i)}x^{\nu(i)}, \tag{3.6}$$

where ν ranges over all the bijections of I to K and $\bar{\mu}$ ranges over all the (not necessarily bijective) mappings of I to J. If $\bar{\mu}$ is not bijective, there are i_1 and i_2 in I such that $i_1 < i_2$ and $\bar{\mu}(i_1) = \bar{\mu}(i_2)$. For a bijection ν of I to K, let ν' be the bijection of I to K determined by $\nu'(i_1) = \nu(i_2)$, $\varphi'(i_2) = \nu(i_1)$, and $\nu'(i) = \nu(i)$ for $i\neq i_1, i_2$. Then the two terms $\Pi_{i\in I}M^{i}_{\bar{\mu}(i)}N^{\bar{\mu}(i)}_{(i)}x^{\nu(i)}$ and $\Pi_{i\in I}M^{\bar{\mu}(i)}_{\nu'(i)}x^{\nu'(i)}$ in (3.6) cancel in the same way as in the proof of Proposition 3.5. Thus (3.6) is equal to (3.5), establishing the proof of the theorem.

Let I and J be G-sets and K' and J' be subsets of I and J, respectively. Let M be an $I\times J$ matrix. By an $I'\times J'$ *minor matrix* of M we mean the $I'\times J'$ matrix whose (i,j) entry is M^{i}_{j} for $(i,j)\in I'\times J'$. Let $i_0\in I$ and $j_0\in J$. The $(I\setminus\{i_0\})\times(J\setminus\{j_0\})$-minor matrix of M is denoted by $M(i_0,j_0)$. When J is unmixed, we define

$$\sigma(I,J,i_0,j_0) = \sigma(g(j_0), g(I) - g(J) + g(j_0) - g(i_0))$$

$$\times\prod_{i<i_0}\epsilon\sigma(g(i), g(i_0))\cdot\prod_{j<j_0}\epsilon\sigma(g(j_0), g(j)),$$

where ϵ is 1 or -1 according as J is odd or even.

Theorem 3.7. Let M be an unmixed $I\times J$ matrix with $|I| = |J|$. Then we have

$$\sum_{j\in J}\sigma(I,J,i,j)M^{k}_{j}\cdot\det M(i,j) = \delta^{k}_{i}\det M, \tag{3.7}$$

for any $i, k\in I$, where δ is Kronecker's delta.

Proof: When $i = k$ in (3.7), the usual calculation of the terms of $\det M$ containing M^{i}_{j} gives the desired formula. When $i\neq k$, Proposition 3.5 (iii) gives the desired equality.

Corollary 3.8: Let M be an unmixed $I\times J$ matrix with $|I|=|J|$. Then M is invertible if and only if $\det M$ is an invertible element of F. In this case the inverse N of M is a $J\times I$ matrix given by

$$N_i^j=\sigma(I,J,i,j)\cdot\det M(i,j)\cdot(\det M)^{-1}. \tag{3.8}$$

Proof: Suppose that $\det M$ is invertible in F. Then by Theorem 3.7, the matrix N given by (3.8) is a right inverse of M, that is, $MN=E_I$, where E_I is the identity $I\times I$ matrix. By Theorem 3.5 we have $\det M\cdot\det N=1$. Thus $\det N$ is also invertible in F (note that a homogeneous one-sided inverse is a two-sided inverse in a σ-commutative algebra) and hence N has a right inverse M'; $NM'=E_J$. Now we have $M=M(NM')=(MN)M'=M'$ This shows that N is the (two-sided) inverse of M.

An $I\times J$ matrix M is called *square* if $I=I_1\cup I_2$, $J=J_1\cup J_2$, I_1 and J_1 are even, I_2 and J_2 are odd, and $|I_1|=|J_1|$, $|I_2|=|J_2|$. Let A (resp. B C, D) be the $I_1\times J_1$ (resp. $I_1\times J_2$, $I_2\times J_1$, $I_2\times J_2$)-minor matrix of M. In this case we write

$$M=\begin{pmatrix}A & B\\ C & D\end{pmatrix}. \tag{3.9}$$

Definition 3.9: For a square $I\times J$ matrix M over F of the form (3.9), the *superdeterminant* $\operatorname{sdet} M$ of M is defined by

$$\operatorname{sdet} M=\begin{cases}0, & \text{if } \det A \text{ or } \det D \text{ is not invertible,}\\ \sigma(g(J_1)-g(J_2),\,g(J_2)-g(I_2))\\ \quad\times(\det A)(\det(D-CA^{-1}B))^{-1}, & \text{otherwise}\end{cases}$$

Since all the elements of B and C are odd and hence nilpotent, we see that M is invertible if and only if both A and D are invertible. Hence by Corollary 3.8, we have the following.

Proposition 3.10: A square $I\times J$ matrix M over F is invertible if and only if $\operatorname{sdet} M\neq 0$.

Theorem 3.11: Let M be a square $I\times J$ matrix and N be a square $J\times K$ matrix over F. Then we have

$$\operatorname{sdet} MN=\operatorname{sdet} M\cdot\operatorname{sdet} N. \tag{3.10}$$

To prove the theorem we need the following lemma.

Lemma 3.12: Let I be an even G-set and J an odd G-set. Let B be an $I\times J$ matrix and C a $J\times I$ matrix over F. Then we have

$$\det(E_I+BC)\cdot\det(E_J+CB)=1. \tag{3.11}$$

Proof: We first claim that if (3.11) is true for $B=B_1$ and $B=B_2$ (C is arbitrary), then it is true for $B=B_1+B_2$. In fact,

$$\begin{aligned}&\det(E_I+(B_1+B_2)C)\cdot\det(E_J+C(B_1+B_2))\\ &\quad=\det(E_I+B_2C(E_I+B_1C)^{-1})\\ &\qquad\times\det(E_I+B_1C)\cdot\det(E_J+CB_1)\\ &\qquad\times\det(E_J+(E_J+CB_1)^{-1}CB_2)=1.\end{aligned}$$

Therefore to prove the lemma, we may assume that only a single (i_0,j_0)-entry of B is nonzero. Then an easy calculation shows $\det(E_I+BC)=1+B^{i_0}_{j_0}C^{j_0}_{i_0}$ and $\det(E_J+CB)=1+C^{j_0}_{i_0}B^{i_0}_{j_0}$. Since $B^{i_0}_{j_0}C^{j_0}_{i_0}=-C^{j_0}_{i_0}B^{i_0}_{j_0}$ and $(B^{i_0}_{j_0}C^{j_0}_{i_0})^2=0$, we find $\det(E_I+BC)\cdot\det(E_J+CB)=1$.

Proof of Theorem 3.11: Let

$$M=\begin{pmatrix}A & B\\ C & D\end{pmatrix}\quad\text{and}\quad N=\begin{pmatrix}X & Y\\ Z & W\end{pmatrix}.$$

We may assume that A, D, X, and W are all invertible; otherwise both sides of (3.10) are 0 by the remark before Proposition 3.10. First assume $Z=0$, then

$$\begin{aligned}\operatorname{sdet} MN&=\epsilon_1\det AX\cdot(\det(CY+DW\\ &\qquad-CX(AX)^{-1}(AY+BW)))^{-1}\\ &=\epsilon_1\det AX\cdot(\det(DW-CA^{-1}BW))^{-1}\\ &=\epsilon_1\det A\cdot\det X\cdot(\det W)^{-1}(\det(D-CA^{-1}B))^{-1}\\ &=\epsilon_1\epsilon_2\det A\cdot(\det(D-CA^{-1}B))^{-1}\cdot\det X\\ &\qquad\times(\det W)^{-1},\end{aligned} \tag{3.12}$$

where $\epsilon_1=\sigma(g(K_1)-g(K_2),\ g(K_2)-g(I_2))$, and $\epsilon_2=\sigma(g(J_1)-g(K_1)-g(J_2)+g(K_2),\ g(J_2)-g(I_2))$. Hence $\epsilon_1\epsilon_2=\sigma(g(J_1)-g(J_2),g(J_2)-g(I_2))\cdot\sigma(g(K_1)-g(K_2),g(K_2)-g(J_2))$. Therefore, (3.12) is equal to $\operatorname{sdet} M\cdot\operatorname{sdet} N$. The case $B=0$ is treated similarly.

Next assume $C=Y=0$. Then, using Lemma 3.12 we have

$$\begin{aligned}\operatorname{sdet} MN&=\epsilon_1\det(AX+BZ)\cdot(\det(DW\\ &\qquad-DZ(AX+BZ)^{-1}BW)))^{-1}\\ &=\epsilon_1\det(AX+BZ)\cdot(\det W)^{-1}\\ &\qquad\times(\det(E_{J_2}-Z(AX+BZ)^{-1}B))^{-1}(\det D)^{-1}\\ &=\epsilon_1\epsilon_2\det(AX+BZ)\cdot\det(E_{K_1}-(AX+BZ)^{-1}BZ)\\ &\qquad\times(\det D)^{-1}(\det W)^{-1}\\ &=\epsilon_1\epsilon_2\det AX\cdot(\det D)^{-1}(\det W)^{-1}\\ &=\epsilon_1\epsilon_2\epsilon_3\det A\cdot(\det D)^{-1}\cdot\det X\cdot(\det W)^{-1},\end{aligned} \tag{3.13}$$

where $\epsilon_1=\sigma(g(K_1)-g(K_2),g(K_2)-g(I_2))$, $\epsilon_2=\sigma(g(K_2)-g(J_2),\ g(J_2)-g(I_2))$, and $\epsilon_3=\sigma(g(J_1)-g(K_1),g(J_2)-g(I_2))$. Thus (3.13) is equal to $\operatorname{sdet} M\cdot\operatorname{sdet} N$. Finally, since

$$\begin{aligned}MN=&\begin{pmatrix}A & 0\\ C & D-CA^{-1}B\end{pmatrix}\cdot\begin{pmatrix}E_{J_1} & A^{-1}B\\ 0 & E_{J_2}\end{pmatrix}\\ &\times\begin{pmatrix}Y & 0\\ Z & W-ZX^{-1}Y\end{pmatrix}\cdot\begin{pmatrix}E_{K_1} & X^{-1}Y\\ 0 & E_{K_2}\end{pmatrix},\end{aligned}$$

the general case can be reduced to the above three cases.

Definition 3.12: For an $I\times J$ matrix M over F, a $(-J)\times(-I)$ matrix M^T called the *supertranspose* of M is defined by

$$M^T{}_i^j=\sigma(g(i),g(j)-g(i))M^i_j.$$

Proposition 3.13: (i) For an $I\times J$ matrix M and a $J\times K$ matrix N, we have

$$(MN)^T=N^TM^T.$$

(ii) For an $I\times I$ matrix M, we have $\operatorname{sdet} M^T=\operatorname{sdet} M$.

Proof: The assertion (i) would be proved by an easy calculation. To prove (ii), let

$$M=\begin{pmatrix}A & B\\ C & D\end{pmatrix}$$

be an $I \times I$ matrix expressed as (3.9). Then

$$M^T = \begin{pmatrix} A^T & C^T \\ B^T & D^T \end{pmatrix}$$

and by (i) we see that A^T (resp. D^T) is invertible if and only if A (resp. D) is invertible. Thus assuming A and D are invertible, we have

$$\begin{aligned} \operatorname{sdet} M^T &= \det A^T \cdot (\det(D^T - B^T (A^T)^{-1} C^T))^{-1} \\ &= \det A^T \cdot (\det(D - CA^{-1}B)^T)^{-1}. \end{aligned}$$

Therefore we may prove (ii) only for an unmixed matrix M. Assume that M is odd (the even case is similar). Let x^i and y^{-i} $(i \in I)$ be indeterminates of grade $g(i)$ and $-g(i)$, respectively, and $k[x, y]$ be the σ-symmetric algebra generated by x^i, y^{-i} $(i \in I)$ over k. In $F[x, y] = F \otimes_k k[x, y]$ we have

$$\begin{aligned} &\det M^T \cdot \prod_{i \in I} x^i \cdot \prod_{-i \in -I} y^{-i} \\ &= \prod_{i \in I} x^i \cdot \det M^T \cdot \prod_{-i \in -I} y^{-i} \\ &= \sum_{\pi} \prod_{i \in I} x^i \cdot \prod_{-i \in -I} \sigma(g(\pi(i)), g(i) - g(\pi(i))) \\ &\quad \times M_i^{\pi(i)} y^{-\pi(i)}, \end{aligned} \tag{3.14}$$

where π ranges over all the bijections of I to I. Since $x^i M_i^{\pi(i)} y^{-\pi(i)}$ is of grade 0 and commutes with any element of $F[x, y]$ and $\sigma(g(\pi(i)), -g(\pi(i))) = \sigma(g(i), -g(i)) = -1$, (3.14) is equal to

$$\begin{aligned} \sum_{\pi} \prod_{i \in I} M^i_{\pi(i)} x^{\pi(i)} y^{-i} &= \sum_{\pi} \prod_{i \in I} M^i_{\pi(i)} x^{\pi(i)} \cdot \prod_{-i \in -I} y^{-i} \\ &= \det M \cdot \prod_{i \in I} x^i \cdot \prod_{-i \in -I} y^{-i}. \end{aligned}$$

It follows that $\det M^T = \det M$.

Definition 3.14: For an $I \times I$ matrix M over F, the *supertrace* $\operatorname{str} M$ is defined by

$$\operatorname{str} M = \sum_{i \in I} \sigma(g(i), g(i)) M^i_i.$$

Proposition 3.15: (i) For an $I \times I$ matrix M, we have $\operatorname{str} M = \operatorname{str} M^T$. (ii) For an $I \times J$ matrix M and $J \times I$ matrix N, we have $\operatorname{str} MN = \operatorname{str} NM$. The proof of Proposition 3.14 is easy and we omit it.

IV. LINEAR LIE GROUPS AND ALGEBRAS WITH σ-SYMMETRIC PARAMETERS

Throughout this section k is the real number field or the complex number field.

Definition 4.1: A G-graded algebra $F = \oplus_{\alpha \in G} F_\alpha$ over k is called a *G-graded Banach algebra*, if it satisfies (i) F_α is a complete normed space for every $\alpha \in G$ (the norm of $a \in F_\alpha$ is written as $\|a\|$); and (ii) for any α, $\beta \in G$ and $a \in F_\alpha$, $b \in F_\beta$, $\|ab\| \leqslant \|a\| \cdot \|b\|$.

Example 4.2: Let x_i $(i \in I)$ be indeterminates of grade $g(i) \in G$ (I is finite or infinite and is linearly ordered). Let $k[x] = k[x_i; i \in I]$ be the σ-symmetric algebra generated by x_i $(i \in I)$ over k. Let $K = \{n_i\}_{i \in I}$ be a sequence of non-negative integers indexed by I such that at most finitely many n_i are positive and that $n_i \leqslant 1$ if $g(i)$ is odd. Then the ordered products $x^K = \Pi_{i \in I} x_i^{n_i}$, where K ranges over all such sequences, form a linear basis of $k[x]$ over k. For a bijection π of I to I we define the number $\sigma(K, \pi)$ by $x^K = \sigma(K, \pi) \Pi_{i \in I} x_{\pi(i)}^{n_{\pi(i)}}$ and set $\delta(K) = \min_\pi |\sigma(K, \pi)|$. We define a norm $\|f(x)\|$ of $f(x) = \Sigma_K a_K x^K \in k[x]$ by

$$\|f(x)\| = \sum_K \delta(K) |a_K|.$$

Let F_α be the completion of $k[x]_\alpha$ for $\alpha \in G$. Then $F = \oplus_{\alpha \in G} F_\alpha$ is a σ-commutative G-graded Banach algebra.

In what follows, F is σ-commutative G-graded Banach algebra over k with identity element 1. Let I and J be G-sets. We define a norm $\|M\|$ of an $I \times J$ matrix M over F by

$$\|M\| = \left(\sum_{i \in I, j \in J} \|M^i_j\|^2 \right)^{1/2}. \tag{4.1}$$

Proposition 4.3: Let M be an $I \times J$ matrix and N be a $J \times K$ matrix over F. Then we have

$$\|MN\| \leqslant \|M\| \cdot \|N\|.$$

F is called *locally finite* if F_α is finite dimensional over k for every $\alpha \in G$. By proposition 4.3 we have the following.

Proposition 4.4: The algebra of $I \times I$ matrices over F is a Banach algebra with the norm (4.1). It is finite dimensional, if F is locally finite.

By the general theory of Banach algebras, we can define the exponential mapping exp on $\mathrm{gl}(I,F)$; for an $I \times I$ matrix M over F we define

$$\exp M = \sum_{n=0}^{\infty} \frac{M^n}{n!}.$$

The following theorem would be proved in a similar way to the usual case, and we omit the proof.

Theorem 4.5: For an $I \times I$ matrix M over F we have

$$\operatorname{sdet}(\exp M) = \exp(\operatorname{str} M).$$

The group of all invertible $I \times I$ matrices M over F forms a topological group with respect to the relative topology in $\mathrm{gl}(I,F)$. It is called the *general linear group of degree I with parameters in F* and is denoted by $\mathrm{GL}(I,F)$.

Let $\mathcal{G}$ be a closed subgroup of $\mathrm{GL}(I,F)$. Define

$$\mathcal{L}(\mathcal{G}) = \{M \in \mathrm{gl}(I,F);\ \exp tM \in \mathcal{G} \text{ for all real numbers } t\}.$$

Then $\mathcal{L}(\mathcal{G})$ forms a Lie subalgebra of $\mathrm{gl}(I,F)$ over the real number field; we call it the *Lie algebra* of $\mathcal{G}$.

Theorem 4.6: Let $\mathcal{G}$ be a closed subgroup of $\mathrm{GL}(I,F)$ and assume that F is locally finite. Then

$$\{\exp X_1 \cdots \exp X_r;\ r \geqslant 1,\ X_i \in \mathcal{L}(\mathcal{G})\}$$

is the connected component of $\mathcal{G}$ containing the identity element of $\mathcal{G}$.

The proof of Theorem 4.6 is also standard. For the general theory of groups embedded in a Banach algebras, we refer to Yoshida.[18]

We give two types of closed subgroups of $\mathrm{GL}(I,F)$. The *special linear group* $\mathrm{SL}(I,F)$ is defined to be the group of those matrices whose superdeterminants are 1. Let Ψ be an invertible $(-I) \times I$ matrix over F. Let $L_\Psi(I,F)$ denote the group of Ψ-preserving $I \times I$ matrices over F, that is,

$$L_\Psi(I,F) = \{M \in \mathrm{GL}(I,F);\ M^T \Psi M = \Psi\}.$$

We define Lie subalgebras $\mathrm{sl}(I,F)$ and $l_\Psi(I,F)$ of $\mathrm{gl}(I,F)$ by

$$\mathrm{sl}(I,F) = \{M \in \mathrm{gl}(I,F); \mathrm{str}\, M = 0\}$$

and

$$l_\Psi(I,F) = \{M \in \mathrm{gl}(I,F); M^T\Psi + \Psi M = 0\}.$$

Easy calculations using Propositions 3.13 and 3.15 show that $L_\Psi(I,F)$ forms a group and $l_\Psi(I,F)$ and $\mathrm{sl}(I,F)$ form Lie algebras.

Proposition 4.7: We have (i) $\mathrm{gl}(I,F) = \mathscr{L}(\mathrm{GL}(I,F))$, (ii) $\mathrm{sl}(I,F) = \mathscr{L}(\mathrm{SL}(I,F))$, and (iii) $l_\Psi(I,F) = \mathscr{L}(L_\Psi(I,F))$.

Proof: (i) is clear, (ii) follows from Theorem 4.5, and (iii) can be proved by using the formula $\Psi(\exp M)\Psi^{-1} = \exp(\Psi M \Psi^{-1})$.

Let $\mathscr{L}$ be a Lie subalgebra of $\mathrm{gl}(I,F)$. Then $\mathscr{L}$ is called *well-parametrized in F*, if there is a free G-graded submodule $\mathbb{L}$ of $\mathbf{gl}(I,F)$ over F such that $\mathscr{L} = \mathrm{gl}(I,F) \cap \mathbb{L}$, in other words, there is a set $\{\mathbf{e}_i\}$ of homogeneous elements of $\mathbf{gl}(I,F)$ such that the $\mathbf{e}_i$'s are linearly independent over F and

$$\mathscr{L} = \oplus_i F_{-g(i)} \cdot \mathbf{e}_i,$$

where $g(i)$ is the grade of $\mathbf{e}_i$. A closed subgroup of $\mathscr{G}$ of $\mathrm{GL}(I,F)$ is called well-parametrized in F, if so is the Lie algebra of $\mathscr{G}$.

The algebras $\mathrm{gl}(I,F)$ and $\mathrm{sl}(I,F)$ are well parametrized. The algebra $l_\Psi(I,F)$ is well parametrized if all the entries of Ψ are in the base field k.

Let $L = \oplus_{\alpha\in G} L_\alpha$ be a G-graded Lie σ-algebra over k (not over F, see Definition 2.5). Assume that L is finite dimensional over k. Then by the generalized Ado theorem (Theorem 3 of Scheunert[14]), L has a faithful graded representation in some finite dimensional G-graded vector space V over k. Let $I = \{i\}$ be a homogeneous basis of V. This I can be considered to be a G-set and L is regarded as a graded subalgebra of $\mathrm{gl}(I,k)$. Let $\mathbb{L} = F \otimes_k L$ and $\mathscr{L} = \oplus_{\alpha\in G}(F_{-\alpha} \otimes_k L_\alpha)$. Then $\mathbb{L}$ and $\mathscr{L}$ are, naturally, subalgebras of $F \otimes_k \mathbf{gl}(I,k) = \mathbf{gl}(I,F)$ and of $\mathrm{gl}(I,F)$, respectively. We clearly have $\mathscr{L} = \mathrm{gl}(I,F) \cap \mathbb{L}$ and so $\mathscr{L}$ is well-parametrized in F. Thus, we have the following.

Proposition 4.7: Let L be a finite-dimensional G-graded Lie σ-algebra over k. Then

$$\mathscr{L} = \oplus_{\alpha\in G}(F_{-\alpha} \otimes_k L_\alpha)$$

is considered to be a well-parametrized Lie subalgebra of $\mathrm{gl}(I,F)$ for a suitable G-set I.

Let L and $\mathscr{L}$ be as in Proposition 4.7. Define

$$\mathscr{G} = \{\exp X_1 \cdots \exp X_r; r \geqslant 1, X_i \in \mathscr{L}\}.$$

Then $\mathscr{G}$ is a subgroup of $\mathrm{GL}(I,F)$. Though $\mathscr{G}$ is not necessarily a closed subgroup, we may be permitted to say that $\mathscr{G}$ is the Lie group with parameters in F associated with L.

V. SUPERIZATION

Let F be a σ-commutative G-graded algebra with 1. In this section G is assumed to be finitely generated.

Let $(\overline{G},\bar{\sigma})$ be the extended signed group defined by (2.7) and (2.8). Define a mapping $\epsilon: G \to Z_2$ by $\epsilon(\alpha) = (1 - \sigma(\alpha,\alpha))/2$ for $\alpha \in G$, that is, $\sigma(\alpha,\alpha) = (-1)^{\epsilon(\alpha)}$. Then ϵ is a homomorphism of groups. Set

$$G' = \{\alpha' = (\alpha, \epsilon(\alpha)); \alpha \in G\},$$

then G' is a subgroup of $\overline{G}$ isomorphic to G. Letting $\sigma' = \bar{\sigma}|_{G'\times G'}$, (G',σ') is an even signed group. By Proposition 2.7 there is a factor system ϕ on G' such that

$$\sigma'(\alpha',\beta') = \phi(\alpha',\beta')/\phi(\beta',\alpha'),$$

for $\alpha',\beta' \in G'$. Let $C = \oplus_{\alpha'\in G'} k \cdot u_{\alpha'}$ be the crossed product of k and G' with respect to the factor system ϕ. Since (G,σ) and (G',σ') are embedded in $(\overline{G},\bar{\sigma})$, F and C are considered to be $\bar{\sigma}$-commutative $\overline{G}$-graded algebras in an obvious way. The graded tensor product $F \otimes_k C$ is a $\bar{\sigma}$-commutative $\overline{G}$-graded algebra and all the (associative) algebras in this section are regarded naturally as its subalgebras. Let $\overline{F}$ be the subalgebra of $F \otimes_k C$ given by

$$\overline{F} = \oplus_{\alpha\in G}(F_\alpha \otimes u_{-\alpha'}),$$

where $\alpha' = (\alpha,\epsilon(\alpha))$. Now $\overline{F}$ is not only a G-graded algebra but also a supercommutative Z_2-graded algebra in the following way. Let us identify the subgroup $\{(0,0),(0,1)\}$ of $\overline{G}$ with Z_2. Since $\alpha + (-\alpha') = (0,\epsilon(\alpha))$, $\overline{F}$ is Z_2-graded algebra with the even component $\oplus_{\alpha\in G_0}(F_\alpha \otimes u_{-\alpha'})$ and the odd component $\oplus_{\alpha\in G_1}(F_\alpha \otimes u_{-\alpha'})$. Since $F \otimes_k C$ is $\bar{\sigma}$-commutative, $\overline{F}$ is supercommutative.

Let I be a G-set. We define a Z_2-set $\overline{I} = \{\bar{i}; i \in I\}$ as follows: $\bar{i} < \bar{j}$ if $i < j$ and $g(\bar{i}) = \epsilon(g(i)) = (0,\epsilon(g(i)))$. Now let U_I be the $I \times \overline{I}$ matrix over $F \otimes_k C$ defined by

$$(U_I)^i_{\bar{j}} = \delta^i_j \otimes u_{g'(i)},$$

for $i,j \in I$, where $g'(i) = (g(i), \epsilon(g(i))) \in G'$. Then U_I is an invertible square matrix satisfying

$$U_I^T \cdot U_{-I} = \Sigma, \tag{5.1}$$

where Σ is a $(-\overline{I}) \times (-\overline{I})$ matrix given by

$$\Sigma^{-\bar{i}}_{-\bar{j}} = \delta^i_j \sigma(g(i), g(i)) \phi(g'(i), -g'(i)) u_0. \tag{5.2}$$

For an $I \times J$ matrix M over F we set

$$\overline{M} = U_I^{-1} M U_J.$$

Here $\overline{M}$ is an $\overline{I} \times \overline{J}$ matrix over $\overline{F}$, that is, a matrix with supersymmetric parameters. We call $\overline{M}$ the *superization* of M. A calculation [using (2.6)] shows

$$\overline{M}^{\bar{i}}_{\bar{j}} = \sigma(g(i), g(j) - g(i))\, \phi(g'(i), g'(j) - g'(i))^{-1} \times M^i_j \otimes u_{g'(j) - g'(i)}. \tag{5.3}$$

The following is easily proved by the definition of superization, Theorem 3.11, and Proposition 3.15.

Proposition 5.1: For an $I \times I$ matrix over F we have

(i) $\mathrm{sdet}\, M = \mathrm{sdet}\, \overline{M}$,

(ii) $\mathrm{str}\, M = \mathrm{str}\, \overline{M}$.

From now on we assume that k is the real or the complex number field and F is a (σ-commutative) G-graded Banach algebra. Moreover, we assume that σ satisfies the condition $|\sigma(\alpha,\beta)| = 1$ for all $\alpha,\beta \in G$. Then, $|\sigma'(\alpha',\beta')| = 1$ for all $\alpha',\beta' \in G'$, and therefore the factor system ϕ also can be chosen so that $|\phi(\alpha',\beta')| = 1$ for all $\alpha',\beta' \in G'$. Thus $\overline{F}$ becomes a G-graded Banach algebra with the norm

$$\|x_\alpha \otimes u_{-\alpha'}\| = \|x_\alpha\|,$$

for $x_\alpha \in F_\alpha$.

Proposition 5.2: For an $I \times I$ matrix M over F we have

$\overline{\exp M} = \exp \overline{M}$.

Definition 5.3: Let $\mathcal{G}$ be a closed subgroup of $G(I,F)$ and $\mathcal{L}$ a Lie subalgebra of $\mathrm{gl}(I,F)$. Then $\overline{\mathcal{G}} = U_I^{-1}\mathcal{G}U_I$ is a closed subgroup of $\mathrm{GL}(\bar{I},\bar{F})$ and $\overline{\mathcal{L}} = U_I^{-1}\mathcal{L}U_I$ a Lie subalgebra of $\mathrm{gl}(\bar{I},\bar{F})$. They are called the *superizations* of $\mathcal{G}$ and $\mathcal{L}$, respectively.

We define $\mathrm{gl}_G(\bar{I},\bar{F})$ to be an algebra of those matrices N in $\mathrm{gl}(\bar{I},\bar{F})$ that satisfy

$$N^{\bar{i}}_{\bar{j}} \in \bar{F}_{g(i)-g(j)} \otimes u_{g'(j)-g'(i)}.$$

In general, for a subset $\mathcal{G}$ of $\mathrm{gl}(\bar{I},\bar{F})$, we write $\mathcal{G}_G$ for $\mathrm{gl}_G(\bar{I},\bar{F}) \cap \mathcal{G}$. For example $\mathrm{sl}_G(\bar{I},\bar{F}) = \mathrm{gl}_G(\bar{I},\bar{F}) \cap \mathrm{sl}(\bar{I},\bar{F})$.

Proposition 5.4: We have

(i) $\overline{\mathrm{gl}(I,F)} = \mathrm{gl}_G(\bar{I},\bar{F})$, $\overline{\mathrm{GL}(I,F)} = GL_G(\bar{I},\bar{F})$,

(ii) $\overline{\mathrm{sl}(I,F)} = \mathrm{sl}_G(\bar{I},\bar{F})$, $\overline{\mathrm{SL}(I,F)} = \mathrm{SL}_G(\bar{I},\bar{F})$,

(iii) $\overline{\mathrm{l}_{(\Psi)}(I,F)} = \mathrm{l}_{\Sigma\bar{\Psi},G}(\bar{I},\bar{F})$, $\overline{\mathrm{L}_{\Psi}(I,F)} = L_{\Sigma\bar{\Psi},G}(\bar{I},\bar{F})$,

where Σ is the $I \times I$ matrix given by (5.2).

Proof: In virtue of (5.3) we readily find

$$\overline{\mathrm{gl}(I,F)} = \mathrm{gl}_G(\bar{I},\bar{F}). \tag{5.4}$$

Next we prove the formula $\overline{l_{\Psi}(I,F)} = l_{\Sigma\bar{\Psi},G}(\bar{I},\bar{F})$. Let $M \in l_{\Psi}(I,F)$, that is, $M^T\Psi + \Psi M = 0$. The last equation is equivalent to

$$U_I^T M^T (U_I^{-1})^T U_I^T (U_{-I})^{-1}\Psi U_I + U_I^T U_{-I}(U_{-I})^{-1}\Psi U_I U_I^{-1} M U_I = 0.$$

Hence by Proposition 3.13 and (5.1) we have

$$\overline{M}^T\Sigma\bar{\Psi} + \Sigma\bar{\Psi}\overline{M} = 0.$$

Therefore, $M \in l_{\Psi}(I,F)$ if an only if $\overline{M} \in l_{\Sigma\bar{\Psi}}(\bar{I},\bar{F})$. This together with (5.4) shows the desired formula. We omit the proof of the other formulas.

By Proposition 5.2 we have the following.

Proposition 5.5: For a closed subgroup of $\mathrm{GL}(I,F)$ we have

$$\overline{\mathcal{L}(\mathcal{G})} = \mathcal{L}(\overline{\mathcal{G}}).$$

Let L be a finite dimensional G-graded Lie σ-algebra over k. As we did in Sec. IV, we regard L as a G-graded subalgebra of $\mathrm{gl}(I,k)$ for a suitable G-set I. $\mathcal{L} = \oplus_{\alpha\in G}(F_{-\alpha} \otimes_k L_\alpha)$ is a subalgebra of $\mathrm{gl}(I,F)$. Let $X \in L$. We define a matrix $\overline{X} \in \mathrm{gl}(\bar{I},k)$ by

$$\overline{X}^{\bar{i}}_{\bar{j}} = \sigma(g(j)-g(i),g(i))\,\phi(g'(j)-g'(i),g'(i))^{-1}X^i_j. \tag{5.5}$$

Now we assume $X \in L_\alpha$ for $\alpha \in G$, and let $f \in F_{-\alpha}$. Then the scalar product $fX = f \otimes X$ defined by (3.1) is in $\mathcal{L}$, and by (5.3) and (5.5) we have

$$\overline{fX} = U_I^{-1} f X U_I = (f \otimes u_{\alpha'})\cdot\overline{X}. \tag{5.6}$$

Here $\overline{X}$ is called the *superization* of X. Moreover, we call $\overline{L} = \{\overline{X}; X \in L\}$ the *superization* of L. As the following proposition shows, $\overline{L}$ is a Lie superalgebra and is essentially Scheunert's superization[14] of L.

Proposition 5.6: $\overline{L}$ is a subalgebra of $\mathrm{gl}(\bar{I},k)$, and so it is a G-graded superalgebra over k.

Proof: Let $\alpha, \beta \in G$ and let $X \in L_\alpha$, $Y \in L_\beta$, $f \in F_{-\alpha}$, and $g \in F_{-\beta}$. We have

$$\begin{aligned} U_I^{-1} fgXYU_I &= \sigma(-\beta,\alpha)U_I^{-1} f X U_I U_I^{-1} g Y U_I \\ &= \sigma(\beta,\alpha)(f \otimes u_{\alpha'})\overline{X}(g \otimes u_{\beta'})\overline{Y} \\ &= (-1)^{\epsilon(\alpha)\epsilon(\beta)}\phi(\alpha',\beta')(fg \otimes u_{\alpha'+\beta'})\overline{XY}. \end{aligned}$$

Similarly we have

$$U_I^{-1} fgYXU_I = (-1)^{\epsilon(\alpha)\epsilon(\beta)}\phi(\beta',\alpha')(fg \otimes u_{\alpha'+\beta'})\overline{YX}.$$

Hence

$$\begin{aligned} (fg \otimes u_{\alpha'+\beta'})\,\overline{\langle X,Y\rangle} &= U_I^{-1} fg\langle X,Y\rangle U_I \\ &= (-1)^{\epsilon(\alpha)\epsilon(\beta)}\phi(\alpha',\beta')(fg \otimes u_{\alpha'+\beta'}) \\ &\quad \times(\overline{XY} - \sigma(\alpha,\beta)\sigma'(\alpha',\beta')^{-1}\overline{YX}) \\ &= (-1)^{\epsilon(\alpha)\epsilon(\beta)}\phi(\alpha',\beta') \\ &\quad \times(fg \otimes u_{\alpha'+\beta'})\langle\overline{X},\overline{Y}\rangle. \end{aligned}$$

Since F can be taken arbitrary, we conclude

$$\langle\overline{X},\overline{Y}\rangle = (-1)^{\epsilon(\alpha)\epsilon(\beta)}\phi(\alpha',\beta')^{-1}\,\overline{\langle X,Y\rangle} \in \overline{L}.$$

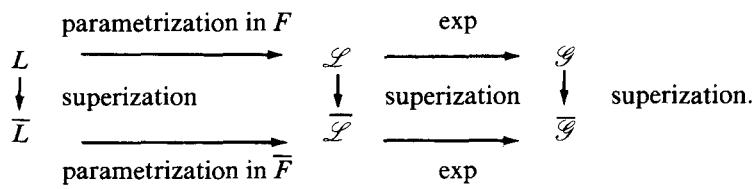
This shows that $\overline{L}$ is a subalgebra of $\mathrm{gl}(\bar{I},k)$.

By (5.6) we have the following.

Proposition 5.7: Under the above situation we have

$$\overline{\oplus_{\alpha\in G}(F_{-\alpha} \otimes_k L_\alpha)} = \oplus_{\alpha\in G}(\overline{F}_{-\alpha} \otimes_k \overline{L}_\alpha).$$

Finally, we summarize the relations between the concepts given in Sec. IV and V in the following diagram:



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Determination of point group harmonics for arbitrary j by a projection method. III. Cubic group, quantization along a ternary axis

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(Received 3 November 1983; accepted for publication 4 May 1984)

The method described in a first paper to obtain cubic harmonics quantized on an axis of order 4 is applied to the case of a ternary quantization axis. Projectors on irreducible representations are expressed with rotation matrices $R(0, \varphi, \pi)$ and $R(\pi, \pi-\varphi, 0)$, $\varphi = \arccos(1/3)$, acting on subspaces of SU(2) invariant under D_3. Relations between the descriptions on the two axes of quantization are derived.

PACS numbers: 02.20. + b, 31.15. + q, 61.50.Em

I. INTRODUCTION

In a previous paper[1] we presented a method for projecting an arbitrary vector of a standard base of group SU(2) on the irreducible representations of the cubic group O_h. We have shown how to build projectors on these representations when the quantization axis $0z$ is an axis of order 4 of the cubic group. It is enough to know the laws of transformation of these representations under the rotation of $\pi/2$ around $0y$ and the reduced matrix elements $d^{(j)}_{mm'}(\pi/2)$. The coefficients of irreducible representations on the standard base of SU(2) can be expressed with these reduced matrix elements together with the square of their norm. The coefficients of normalized representations are square roots of rational numbers. In the case of nondegeneracy, the result does not depend on the choice of the projected vector, except for a sign; in case of degeneracy, after a Schmidt orthogonalization process, the norm is still known without an explicit summation, and the coefficients of orthonormalized representations are also square roots of rational numbers. In a second paper[2] one of us applied this method to the representations of the icosahedral group along an axis of quantization of order 5; in this case, coefficients of representations are linear combinations of two reduced rotation matrices for angles $\beta = \arccos(\pm 1/\sqrt{5})$ which are square roots of rational numbers.

When a physical system invariant under the cubic group is submitted to a perturbation having a ternary symmetry, it is convenient to express the cubic harmonics using the axis of quantization along an axis of order 3. This is the subject of this paper. Such an axis has been chosen very rarely by authors who have given tables.[3–5]

In the second section, we list Euler angles (α, β, γ) of group elements relative to a ternary axis and we give the β dependence of the transformations of irreducible representations. In the third and fourth sections, we derive the projectors on half-integral and integral representations. This question is similar to the case of icosahedral harmonics: a vector $|jm\rangle$ may be the sum of more than two irreducible representations; in one case, it is the sum of two different components of a similar kind of representation.

In Sec. V, we derive the coefficients along a ternary axis of cubic harmonics whose coefficients along a quarternary axis are known, and vice versa. For multidimensional representations, since coefficients of different components are strongly related, it is possible to express ternary coefficients of all components using quaternary coefficients of an arbitrary component. The last section shows that both matrix elements of projectors and coefficients of transformations between ternary and quaternary description are square roots of rational numbers.

II. REPRESENTATIONS OF THE CUBIC GROUP WITH A TERNARY AXIS OF QUANTIZATION

As $0xyz$ is the direct reference frame defined by three axes of order 4, we choose the ternary axis of quantization $0Z$ in the first octant and the twofold symmetry axis $0Y$ as the second bisectrix of the $0xy$ plane:

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} 1/\sqrt{6} & 1/\sqrt{6} & -\sqrt{\frac{2}{3}} \\ -1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{1}$$

The two rotations of $2\pi/3$ around $0Z$ and $\pi/4$ around $0y$, whose Euler angles (α, β, γ) relatively to $0XYZ$ are, respectively, $(0, 0, 2\pi/3)$ and $(2\pi/3, \varphi, 5\pi/3)$, $\varphi = \arccos(1/3)$, are a system of generators of the group, whose 24 elements have the following Euler angles:

$$\alpha = 0, \quad \beta = 0, \pi, \quad \gamma = 0, 2\pi/3, 4\pi/3, \tag{2a}$$

$$\alpha = 0, 2\pi/3, 4\pi/3, \ \beta = \arccos(1/3), \ \gamma = \pi/3, \pi, 5\pi/3, \tag{2b}$$

$$\alpha = \pi/3, \pi, 5\pi/3, \ \beta = \arccos(-1/3), \ \gamma = 0, 2\pi/3, 4\pi/3. \tag{2c}$$

The double cubic group is obtained by adding to that list the 24 elements derived by addition of 2π to α.

An arbitrary group element is represented, in the basis of vectors $|jm\rangle$ of an irreducible representation $\mathscr{D}_j$ of SU(2), by the rotation matrix having the corresponding Euler angles. Our reference frame $0XYZ$ has been chosen so that the representative matrices of the two nontrivial rotations we will have to deal with, i.e., $R(0, \varphi, \pi)$ and $R(\pi, \pi - \varphi, 0)$, are

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symmetric, real for integer values of j, purely imaginary for half-integer values of j.

The six elements (2a) define what is called the D_3 group. Let us introduce the subspaces of $\mathscr{D}_j$ which are invariant under D_3.

For integer values of j, there are four:

$$|j\,\hat{0}\pm\rangle = \left\{ |jm\pm\rangle = \frac{1}{\sqrt{2(1+\delta_{m,0})}} \times(|jm\rangle \pm (-1)^{j-m}|j-m\rangle), \quad \begin{matrix} m>0 \\ m\equiv 0(3) \end{matrix} \right\},$$
$$|j\pm\hat{1}\rangle = \{|jm\rangle,\ m\equiv\pm 1(3)\}. \tag{3}$$

For half-integer values of j there are three:

$$|j\pm\hat{\tfrac{1}{2}}\rangle = \{|jm\rangle,\quad m\equiv\pm\tfrac{1}{2}(3)\},$$
$$|j\,\hat{\tfrac{3}{2}}\rangle = \{|jm\rangle,\ m\equiv\tfrac{3}{2}(3)\}. \tag{4}$$

For integer values of j, among the five irreducible representations Γ_1 to Γ_5, two of them, Γ_1 and Γ_4, behave like $\mathscr{D}_0$ and $\mathscr{D}_1$, respectively, and we identify their components $|\Gamma_i\,\hat{m}\rangle$ with the corresponding standard vectors $|jm\rangle$. Representation $\mathscr{D}_2$ decomposes into $\Gamma_3+\Gamma_5$, and $\mathscr{D}_3$ into $\Gamma_2+\Gamma_4+\Gamma_5$. We choose

$$\begin{aligned}
&|\Gamma_3\pm\hat{1}\rangle = (1/\sqrt{3})|2\mp 2\rangle \pm\sqrt{\tfrac{2}{3}}|2\pm 1\rangle,\\
&|\Gamma_5\,\hat{0}\rangle = |2\,0\rangle,\\
&|\Gamma_5\pm\hat{1}\rangle = -(1/\sqrt{3})|2\pm 1\rangle \pm\sqrt{\tfrac{2}{3}}|2\mp 2\rangle,\\
&|\Gamma_2\,\hat{0}\rangle = (\sqrt{5}/3)|3\,0\rangle + \tfrac{2}{3}(1/\sqrt{2})(|3\,3\rangle - |3\,-3\rangle).
\end{aligned} \tag{5}$$

The behavior of these five representations under a rotation of $2\pi/3$ around $0Z$ and of π around $0Y$ allows us to determine which subspaces of D_3 contribute to a given component of a given representation (see Table I).

Under the rotation $R_Y = R(0,\pi,0)$ of π around $0Y$, the laws of transformation are

$$\begin{aligned}
&|\Gamma_1\,\hat{0}\rangle\to|\Gamma_1\,\hat{0}\rangle,\\
&|\Gamma_2\,\hat{0}\rangle\to-|\Gamma_2\,\hat{0}\rangle,\\
&|\Gamma_3\pm\hat{1}\rangle\to|\Gamma_3\mp 1\rangle,\\
&|\Gamma_4\pm\hat{1}\rangle\to|\Gamma_4\mp\hat{1}\rangle,\\
&|\Gamma_4\,\hat{0}\rangle\to-|\Gamma_4\,\hat{0}\rangle,\\
&|\Gamma_5\pm\hat{1}\rangle\to-|\Gamma_5\mp\hat{1}\rangle,\\
&|\Gamma_5\,\hat{0}\rangle\to|\Gamma_5\,\hat{0}\rangle.
\end{aligned} \tag{6}$$

These laws are different from the corresponding laws for a quarternary axis [formula (4) in Ref. 1] because $0Y$ is a twofold axis for the cube and $0y$ is a fourfold axis.

Under the two rotations $R_1 = R(0,\varphi,\pi)$, $R_2 = R(\pi,\pi-\varphi,0)$, whose product is $R_1R_2 = R_2R_1 = R(0,\pi,0)$, the laws of transformation are (we use $\epsilon = 1$ for R_1, $\epsilon = -1$ for R_2)

$$\begin{aligned}
&|\Gamma_1\,\hat{0}\rangle\to|\Gamma_1\,\hat{0}\rangle,\\
&|\Gamma_2\,\hat{0}\rangle\to-\epsilon|\Gamma_2\,\hat{0}\rangle,\\
&|\Gamma_3\pm\hat{1}\rangle\to|\Gamma_3\mp\hat{\epsilon}\rangle,
\end{aligned}$$

TABLES I and II. Correspondence between irreducible representations of O_h and subspaces adapted to D_3. Each of the subspaces adapted to the irreducible representations of D_3, listed in the first column, is the direct sum of those subspaces of irreducible representations of O_h which are listed in its row. The first row contains two notations: the one used in the present paper, adapted from Bethe, and the one defined by Placzek and more widely known as the Mulliken notation (see Ref. 1 for references). Our notation is chosen as follows: $|\Gamma_i\,\hat{p}\rangle$ notes a component p of a representation Γ_i, $i=1,\ldots,8$, which behaves under a rotation of D_3 like its associated base vectors listed in (3) and (4).

TABLE I.

D_3 \ O	Γ_1 A_1	Γ_2 A_2	Γ_3 E	Γ_4 T_1	Γ_5 T_2
$\|\hat{0}+\rangle$	$\|\Gamma_1\,\hat{0}\rangle$				$\|\Gamma_5\,\hat{0}\rangle$
$\|\hat{0}-\rangle$		$\|\Gamma_2\,\hat{0}\rangle$		$\|\Gamma_4\,\hat{0}\rangle$	
$\|\hat{1}\rangle$			$\|\Gamma_3\,\hat{1}\rangle$	$\|\Gamma_4\,\hat{1}\rangle$	$\|\Gamma_5\,\hat{1}\rangle$
$\|-\hat{1}\rangle$			$\|\Gamma_3-\hat{1}\rangle$	$\|\Gamma_4-\hat{1}\rangle$	$\|\Gamma_5-\hat{1}\rangle$

TABLE II.

D_3 \ O^+	Γ_6 E'	Γ_7 E''	Γ_8 U'
$\|\frac{3}{2}\rangle$			$\|\Gamma_8\,\frac{3}{2}\rangle$, $\|\Gamma_8-\frac{3}{2}\rangle$
$\|\frac{1}{2}\rangle$	$\|\Gamma_6\,\frac{1}{2}\rangle$	$\|\Gamma_7\,\frac{1}{2}\rangle$	$\|\Gamma_8\,\frac{1}{2}\rangle$
$\|-\frac{1}{2}\rangle$	$\|\Gamma_6-\frac{1}{2}\rangle$	$\|\Gamma_7-\frac{1}{2}\rangle$	$\|\Gamma_8-\frac{1}{2}\rangle$

$$\begin{pmatrix}|\Gamma_4\ \ \hat{1}\rangle\\ |\Gamma_4\ \ \hat{0}\rangle\\ |\Gamma_4\ -\hat{1}\rangle\end{pmatrix}\to\frac{1}{3}\begin{pmatrix}-\frac{3+\epsilon}{2} & -2\epsilon & -\frac{3-\epsilon}{2}\\ -2\epsilon & \epsilon & 2\epsilon\\ -\frac{3-\epsilon}{2} & 2\epsilon & -\frac{3+\epsilon}{2}\end{pmatrix}\times\begin{pmatrix}|\Gamma_4\ \ \hat{1}\rangle\\ |\Gamma_4\ \ \hat{0}\rangle\\ |\Gamma_4\ -\hat{1}\rangle\end{pmatrix} \tag{7}$$

$$\begin{pmatrix}|\Gamma_5\ \ \hat{1}\rangle\\ |\Gamma_5\ \ \hat{0}\rangle\\ |\Gamma_5\ -\hat{1}\rangle\end{pmatrix}\to\frac{1}{3}\begin{pmatrix}\frac{1+3\epsilon}{2} & 2 & -\frac{1+3\epsilon}{2}\\ 2 & -1 & -2\\ -\frac{1+3\epsilon}{2} & -2 & \frac{1+3\epsilon}{2}\end{pmatrix}\times\begin{pmatrix}|\Gamma_1\ \ \hat{1}\rangle\\ |\Gamma_5\ \ \hat{0}\rangle\\ |\Gamma_5\ -\hat{1}\rangle\end{pmatrix}.$$

For half-integer values of j, among the three additional irreducible representations Γ_6 to Γ_8, two of them, Γ_6 and Γ_8, behave like $\mathscr{D}_{1/2}$ and $\mathscr{D}_{3/2}$, respectively, and we identify

their components $|\Gamma_i\,\hat{m}\rangle$ with the corresponding standard vectors $|j\,m\rangle$. Representation $\mathscr{D}_{5/2}$ decomposes into $\Gamma_7+\Gamma_8$, and we choose

$$|\Gamma_7\ \pm\hat{\tfrac{1}{2}}\rangle=(\sqrt{5}/3)|\tfrac{5}{2}\ \pm\tfrac{1}{2}\rangle\mp\tfrac{2}{3}|\tfrac{5}{2}\ \mp\tfrac{5}{2}\rangle. \tag{8}$$

Subspaces of D_3 which contribute to a given component of a given representation are listed in Table II. Under the rotation $R\,(0,\pi,0)$ of π around $0Y$, the laws of transformation are

$$\begin{aligned}
&|\Gamma_6\ \pm\hat{\tfrac{1}{2}}\rangle\to\pm\,|\Gamma_6\ \mp\hat{\tfrac{1}{2}}\rangle,\\
&|\Gamma_7\ \pm\hat{\tfrac{1}{2}}\rangle\to\pm\,|\Gamma_7\ \mp\hat{\tfrac{1}{2}}\rangle,\\
&|\Gamma_8\ \pm\hat{\tfrac{3}{2}}\rangle\to\pm\,|\Gamma_8\ \mp\hat{\tfrac{3}{2}}\rangle,\\
&|\Gamma_8\ \pm\hat{\tfrac{1}{2}}\rangle\to\mp\,|\Gamma_8\ \mp\hat{\tfrac{1}{2}}\rangle.
\end{aligned} \tag{9}$$

Representative matrices of transformations $R_1=iR\,(0,\varphi,\pi)$, $R_2=iR\,(\pi,\pi-\varphi,0)$ are real symmetric for half-integer values of j, and representations transform under R_1 like

$$\begin{pmatrix}|\Gamma_6\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_6\ -\hat{\frac{1}{2}}\rangle\end{pmatrix}\to\frac{1}{\sqrt{3}}\begin{pmatrix}\sqrt{2}&1\\1&-\sqrt{2}\end{pmatrix}\begin{pmatrix}|\Gamma_6\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_6\ -\hat{\frac{1}{2}}\rangle\end{pmatrix},$$

$$\begin{pmatrix}|\Gamma_7\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_7\ -\hat{\frac{1}{2}}\rangle\end{pmatrix}\to\frac{1}{\sqrt{3}}\begin{pmatrix}-\sqrt{2}&1\\1&\sqrt{2}\end{pmatrix}\begin{pmatrix}|\Gamma_7\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_7\ -\hat{\frac{1}{2}}\rangle\end{pmatrix}, \tag{10}$$

$$\begin{pmatrix}|\Gamma_8\,\hat{\frac{3}{2}}\rangle\\ |\Gamma_8\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_8\ -\hat{\frac{1}{2}}\rangle\\ |\Gamma_8\ -\hat{\frac{3}{2}}\rangle\end{pmatrix}$$

$$\to\frac{1}{3\sqrt{3}}\begin{pmatrix}-2\sqrt{2}&-2\sqrt{3}&-\sqrt{6}&-1\\-2\sqrt{3}&0&3&\sqrt{6}\\-\sqrt{6}&3&0&-2\sqrt{3}\\-1&\sqrt{6}&-2\sqrt{3}&2\sqrt{2}\end{pmatrix}$$

$$\times\begin{pmatrix}|\Gamma_8\,\hat{\frac{3}{2}}\rangle\\ |\Gamma_8\,\hat{\frac{1}{2}}\rangle\\ |\Gamma_8\ -\hat{\frac{1}{2}}\rangle\\ |\Gamma_8\ -\hat{\frac{3}{2}}\rangle\end{pmatrix}.$$

The transformation law of Γ_i, $i=6,7,8$, under R_2 follows from the relation

$$(R_{2,i})_{m,m'}=(R_{1,i})_{m,m'}(-1)^{j_i-m}, \tag{11}$$

with $j_6=j_7=\frac{1}{2}, j_8=\frac{3}{2}$.

Due to parity properties under the action of $R_Y=R\,(0,\pi,0)$, we will consider only components $|\Gamma_i\,\hat{m}\rangle$ with nonnegative values of $\hat{m}$.

III. PROJECTION OF A VECTOR $|jm\rangle$ ON AN IRREDUCIBLE REPRESENTATION OF THE DOUBLE CUBIC GROUP FOR HALF-INTEGER VALUES OF j

Two qualitative differences exist with the case of a quaternary axis of quantization.[1] First, an arbitrary vector $|jm\rangle$ of one of subspaces (4) is the sum of at most three, and not merely two, unnormalized vectors belonging to $|\Gamma_i\,\hat{m}\rangle$ subspaces; this implies that we need two group elements, not merely one, in order to express projectors. Second, subspace $|j\,\hat{\frac{3}{2}}\rangle$ is invariant under $R\,(0,\pi,0)$ on the contrary of subspaces $|j\ \pm\hat{\frac{1}{2}}\rangle$ which are exchanged, and any vector in it is the sum of two unnormalized vectors belonging to $|\Gamma_8\,\hat{\frac{3}{2}}\rangle$ and to $|\Gamma_8\ -\hat{\frac{3}{2}}\rangle$ subspaces. These two features also appear for the icosahedral group,[2] and the method we follow is quite similar to that case.

Let us consider a vector $|jm\rangle$ of subspace $|j\,\hat{\frac{1}{2}}\rangle$:

$$m\equiv\tfrac{1}{2}(3):|jm\rangle=|\Gamma_6\,\hat{\tfrac{1}{2}}\rangle_m+|\Gamma_7\,\hat{\tfrac{1}{2}}\rangle_m+|\Gamma_8\,\hat{\tfrac{1}{2}}\rangle_m, \tag{12}$$

where the subscript m reminds us that the vector is unnormalized and depends on m. The action of $R_1=iR\,(0,\varphi,\pi)$ on $|j\,m\rangle$ yields

$$\begin{aligned}
m\equiv\frac{1}{2}(3):R_1|jm\rangle&=(-1)^{1/2-m}\sum_{m'}d^{(j)}_{m'm}(\varphi)|jm'\rangle\\
&=\frac{\sqrt{2}}{\sqrt{3}}|\Gamma_6\,\hat{\tfrac{1}{2}}\rangle_m+\frac{1}{\sqrt{3}}|\Gamma_6\ -\hat{\tfrac{1}{2}}\rangle_m\\
&\quad-\frac{\sqrt{2}}{\sqrt{3}}|\Gamma_7\,\hat{\tfrac{1}{2}}\rangle_m+\frac{1}{\sqrt{3}}|\Gamma_7\ -\hat{\tfrac{1}{2}}\rangle_m-\frac{2}{3}|\Gamma_8\,\hat{\tfrac{3}{2}}\rangle_m\\
&\quad+\frac{1}{\sqrt{3}}|\Gamma_8\ -\hat{\tfrac{1}{2}}\rangle_m+\frac{\sqrt{2}}{3}|\Gamma_8\ -\hat{\tfrac{3}{2}}\rangle_m,
\end{aligned} \tag{13}$$

and the action of $R_2=iR\,(\pi,\pi-\varphi,0)$ on $|j\,m\rangle$ yields

$$\begin{aligned}
m\equiv\frac{1}{2}(3):R_2|jm\rangle&=\sum_{m'}(-1)^{1/2-m'}d^{(j)}_{m'm}(\pi-\varphi)|jm'\rangle\\
&=\frac{1}{\sqrt{3}}|\Gamma_6\,\hat{\tfrac{1}{2}}\rangle_m-\frac{\sqrt{2}}{\sqrt{3}}|\Gamma_6\ -\hat{\tfrac{1}{2}}\rangle_m\\
&\quad+\frac{1}{\sqrt{3}}|\Gamma_7\,\hat{\tfrac{1}{2}}\rangle_m+\frac{\sqrt{2}}{\sqrt{3}}|\Gamma_7\ -\hat{\tfrac{1}{2}}\rangle_m+\frac{\sqrt{2}}{3}|\Gamma_8\,\hat{\tfrac{3}{2}}\rangle_m\\
&\quad-\frac{1}{\sqrt{3}}|\Gamma_8\,\hat{\tfrac{1}{2}}\rangle_m+\frac{2}{3}|\Gamma_8\ -\hat{\tfrac{3}{2}}\rangle_m.
\end{aligned} \tag{14}$$

Equations (12)–(14) give projections of representations from subspace $|j\,\hat{\frac{1}{2}}\rangle$ to subspaces $|j\ \pm\hat{\frac{1}{2}}\rangle$, $|j\,\hat{\frac{3}{2}}\rangle$. Indeed, beginning with nondiagonal projections, elimination of $|\Gamma_8\ -\hat{\frac{3}{2}}\rangle_m$ between (13) and (14) leads to

$$m\equiv\tfrac{1}{2}(3):|\Gamma_8\,\hat{\tfrac{3}{2}}\rangle_m=\frac{1}{\sqrt{2}}\sum_{m'\equiv 3/2(3)}\{-(-1)^{1/2-m}\sqrt{2}\,d^{(j)}_{m'm}(\varphi)+(-1)^{1/2-m'}d^{(j)}_{m'm}(\pi-\varphi)\}|jm'\rangle. \tag{15}$$

As for diagonal projections, elimination of two of the three components $|\Gamma_i\,\hat{\frac{1}{2}}\rangle$, $i=6,7,8$ between (12), (13), and (14) yields the projector on the third one:

$$m\equiv\frac{1}{2}(3):|\Gamma_6\,\hat{\tfrac{1}{2}}\rangle_m=\frac{1}{4}\sum_{m'\equiv 1/2(3)}\{\delta_{m'm}+\sqrt{6}(-1)^{1/2-m}d^{(j)}_{m'm}(\varphi)+\sqrt{3}(-1)^{1/2-m'}d^{(j)}_{m'm}(\pi-\varphi)\}|jm'\rangle \tag{16}$$

$$|\Gamma_7\,\hat{\tfrac{1}{2}}\rangle_m=\frac{1}{4}\sum_{m'\equiv 1/2(3)}\{\delta_{m'm}-\sqrt{6}(-1)^{1/2-m}d^{(j)}_{m'm}(\varphi)+\sqrt{3}(-1)^{1/2-m'}d^{(j)}_{m'm}(\pi-\varphi)\}|jm'\rangle \tag{17}$$

$$|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_m = \frac{1}{2} \sum_{m' \equiv 1/2(3)} \{\delta_{m'm} - \sqrt{3}(-1)^{1/2-m'} d^{(j)}_{m'm}(\pi - \varphi)\} |jm'\rangle. \tag{18}$$

For subspace $|j \hat{\tfrac{3}{2}}\rangle$, we must take care that an an arbitrary vector $|jm\rangle$ of that subspace is the sum of two distinct kinds of unnormalized components of Γ_8 or more precisely

$$m \equiv \tfrac{3}{2}(3): \quad |jm\rangle = |\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m + |\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_{-m} \tag{19}$$

$$|j \; -m\rangle = (-1)^{j-m}(|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_m - |\Gamma_8 \hat{\tfrac{3}{2}}\rangle_{-m}). \tag{20}$$

The two vectors $|jm\rangle$ and $|j \; -m\rangle$ are related by a rotation of π round the $0Y$ axis, and the two representations $|\Gamma_8\rangle_m$ and $|\Gamma_8\rangle_{-m}$ are different: $|\Gamma_8\rangle_m$ is the one for which the vector $|\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m$ can be projected from $|jm\rangle$ and $|\Gamma_8\rangle_{-m}$ the one for which the vector $|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_{-m}$ can be projected from the same vector $|jm\rangle$.

The action of R_1 and R_2 on Eq. (19) yields

$$\begin{aligned} m \equiv \frac{3}{2}(3): R_1|jm\rangle &= (-1)^{1/2-m} \sum_{m'} d^{(j)}_{m'm}(\varphi)|jm'\rangle \\ &= \frac{1}{3\sqrt{3}} \left(-2\sqrt{2}|\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m - 2\sqrt{3}|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_m - \sqrt{6}|\Gamma_8 \; -\hat{\tfrac{1}{2}}\rangle_m - |\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_m \right. \\ &\quad \left. - |\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m + \sqrt{6}|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_{-m} - 2\sqrt{3}|\Gamma_8 \; -\hat{\tfrac{1}{2}}\rangle_{-m} + 2\sqrt{2}|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_{-m} \right), \end{aligned} \tag{21}$$

$$\begin{aligned} m \equiv \frac{3}{2}(3): R_2|jm\rangle &= \sum_{m'} (-1)^{1/2-m'} d^{(j)}_{m'm}(\pi - \varphi)|jm'\rangle \\ &= \left(\frac{1}{3\sqrt{3}}\right)\left(-|\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m + \sqrt{6}|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_m - 2\sqrt{3}|\Gamma_8 \; -\hat{\tfrac{1}{2}}\rangle_m + 2\sqrt{2}|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_m \right. \\ &\quad \left. + 2\sqrt{2}|\Gamma_8 \hat{\tfrac{3}{2}}\rangle_{-m} + 2\sqrt{3}|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_{-m} + \sqrt{6}|\Gamma_8 \; -\hat{\tfrac{1}{2}}\rangle_{-m} + |\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_{-m} \right). \end{aligned} \tag{22}$$

Elimination of $|\Gamma_8 \hat{\tfrac{1}{2}}\rangle_{-m}$ between (21) and (22) gives the projector from $|j \hat{\tfrac{3}{2}}\rangle$ subspace to $|j \hat{\tfrac{1}{2}}\rangle$ subspace

$$m \equiv \frac{3}{2}(3): |\Gamma_8 \hat{\tfrac{1}{2}}\rangle_m = \frac{1}{\sqrt{2}} \sum_{m' \equiv 1/2(3)} \{ -\sqrt{2}(-1)^{1/2-m} d^{(j)}_{m'm}(\varphi) + (-1)^{1/2-m'} d^{(j)}_{m'm}(\pi - \varphi)\} |jm'\rangle. \tag{23}$$

Elimination of $|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_m$, $|\Gamma_8 \; -\hat{\tfrac{3}{2}}\rangle_{-m}$ and therefore $|\Gamma_8 \hat{\tfrac{3}{2}}\rangle_{-m}$ between (19), (21), and (22) gives the restriction of projector on $|\Gamma_8 \hat{\tfrac{3}{2}}\rangle$ to subspace $|j \hat{\tfrac{3}{2}}\rangle$:

$$m \equiv \frac{3}{2}(3): |\Gamma_8 \hat{\tfrac{3}{2}}\rangle_m = \frac{1}{2} \sum_{m' \equiv 3/2(3)} \left\{ \delta_{m'm} - \frac{2\sqrt{2}}{\sqrt{3}}(-1)^{1/2-m} d^{(j)}_{m'm}(\varphi) - \frac{1}{\sqrt{3}}(-1)^{1/2-m'} d^{(j)}_{m'm}(\pi - \varphi) \right\} |jm'\rangle. \tag{24}$$

Expressions for projections (15)–(18), (23), and (24) simplify greatly if, instead of using matrices $d^{(j)}(\varphi)$ and $d^{(j)}(\pi - \varphi)$, we take the two following matrices:

$$\begin{aligned} A^{(j)}_{m'm} &= \tfrac{1}{4}\{(-1)^{1/2-m'} \cos(\varphi/2) d^{(j)}_{m'm}(\varphi) \\ &\quad + (-1)^{1/2-m} \sin(\varphi/2) d^{(j)}_{m'm}(\pi - \varphi)\}, \end{aligned} \tag{25}$$

$$\begin{aligned} B^{(j)}_{m'm} &= \tfrac{1}{4}\{(-1)^{1/2-m'} \cos(\varphi/2) d^{(j)}_{m'm}(\varphi) \\ &\quad - (-1)^{1/2-m} \sin(\varphi/2) d^{(j)}_{m'm}(\pi - \varphi)\}. \end{aligned}$$

These matrices have a better structure (see Sec. V) and the projectors are, respectively,

$$\begin{aligned} P_6 &= \tfrac{1}{4} + A && |j \hat{\tfrac{1}{2}}\rangle, \\ P_7 &= \tfrac{1}{4} - B && |j \hat{\tfrac{3}{2}}\rangle, \\ P_8 &= \begin{pmatrix} \tfrac{1}{2} - A - B/3 & -(2\sqrt{2}/\sqrt{3})B \\ -(2\sqrt{2}/\sqrt{3})B & \tfrac{1}{2} - A + B \end{pmatrix} && \begin{matrix} |j \hat{\tfrac{3}{2}}\rangle, \\ |j \hat{\tfrac{1}{2}}\rangle. \end{matrix} \end{aligned} \tag{26}$$

In these expressions, subspaces of D_3 are indicated on the right, zero matrix elements are not written, and the first column of P_8 deals with the $|\Gamma_8 \hat{\tfrac{3}{2}}\rangle$ vector.

IV. PROJECTION OF A VECTOR $|jm\rangle$ ON AN IRREDUCIBLE REPRESENTATION OF THE CUBIC GROUP FOR INTEGER VALUES OF j

As seen in Table I, any vector of subspaces $|\hat{0} \; +\rangle$ and $|\hat{0} \; -\rangle$ can be projected on two irreducible representations of the cubic group and any vector of the two other subspaces has projections on three irreducible representations. We no longer have the favorable cases of a quaternary axis of quantization, where the number of Γ_4 (resp. Γ_5) was equal to the dimension of subspace $|\hat{0} \; -\rangle$ (resp. $|\hat{2} \; -\rangle$), thus leading to a natural choice.

Considering an arbitrary vector $|jm \; +\rangle$ of subspace $|j\hat{0} \; +\rangle$ as defined by (3), we write it as the sum of two unnormalized vectors:

$$m \equiv 0 \; (3): \; |jm \; +\rangle = |\Gamma_1 \hat{0}\rangle_m + |\Gamma_5 \hat{0}\rangle_m. \tag{27}$$
$$m \geqslant 0$$

The action of $R_1 = R(0, \varphi, \pi)$ gives

$$m\equiv 0\ (3):\ R_1|jm\ +\rangle = \frac{1}{\sqrt{2(1+\delta_{m0})}}\left\{\sum_{\substack{m'\equiv 0(3)\\ m'>0}} \frac{2}{\sqrt{2(1+\delta_{m'0})}}\left[(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\right]|jm'\ +\rangle\right.$$
$$\left. +\sum_{m'\not\equiv 0(3)}\left[(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\right]|jm'\rangle\right\}$$
$$= |\Gamma_1\,\hat{0}\rangle_m + \tfrac{2}{3}|\Gamma_5\,\hat{1}\rangle_m - \tfrac{1}{3}|\Gamma_5\,\hat{0}\rangle_m - \tfrac{2}{3}|\Gamma_5\ -\hat{1}\rangle_m. \tag{28}$$

Equations (27) and (28) give representations $|\Gamma_1\,\hat{0}\rangle$ and the three components of Γ_5. Indeed, (28) gives the nondiagonal projection of $|\Gamma_5\,\hat{1}\rangle$:

$$m\equiv 0\ (3):|\Gamma_5\,\hat{1}\rangle_m = \frac{3}{2}\sum_{m'\equiv 1(3)}\left[(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\right]|jm'\rangle. \tag{29}$$

The components $|\Gamma_1\,\hat{0}\rangle$ and $|\Gamma_5\,\hat{0}\rangle$ are obtained by elimination of, respectively, $|\Gamma_5\,\hat{0}\rangle$ and $|\Gamma_1\,\hat{0}\rangle$ between (27) and (28):

$$m\equiv 0\ (3):|\Gamma_1\,\hat{0}\rangle = \frac{1}{4}\sum_{\substack{m'\equiv 0(3)\\ m'>0}}\left\{\delta_{m'm}+\frac{3}{\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}}\right.$$
$$\left.\times\left[(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\right]\right\}|jm'\ +\rangle, \tag{30}$$

$$m\equiv 0\ (3):|\Gamma_5\,\hat{0}\rangle_m = \frac{3}{4}\sum_{\substack{m'\equiv 0(3)\\ m'>0}}\left\{\delta_{m'm}+\frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}}\right.$$
$$\left.\times\left[(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\right]\right\}|jm'\ +\rangle. \tag{31}$$

If we had used $R_2 = R(\pi, \pi-\varphi, 0)$ instead of R_1 in order to split the two terms of Eq. (27), we would of course have obtained exactly the same expressions (29)–(31) which mix reduced matrix elements for angles φ and $\pi-\varphi$.

Projections of vectors of subspaces $|j\hat{0}\ -\rangle$ and $|j\ \hat{1}\rangle$ are obtained in a similar way, and we just list the results below, expressed with the two following real, symmetric matrices:

$$C^{(j)}_{m'm} = \frac{3}{4\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}}$$
$$\times\{(-1)^m d^{(j)}_{m'm}(\varphi)+(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\},$$
$$D^{(j)}_{m'm} = \frac{3}{4\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}}$$
$$\times\{(-1)^m d^{(j)}_{m'm}(\varphi)-(-1)^{m'} d^{(j)}_{m'm}(\pi-\varphi)\}, \tag{32}$$

$$P_1 = \tfrac{1}{4}+C \qquad |j\hat{0}\ +\rangle, \tag{33a}$$
$$P_2 = \tfrac{1}{4}-D \qquad |j\hat{0}\ -\rangle, \tag{33b}$$
$$P_3 = \tfrac{1}{4}+(C-D)/2 \qquad |j\hat{1}\rangle, \tag{33c}$$
$$P_4 = \begin{pmatrix} \tfrac{3}{8}-\tfrac{3}{4}C-D/4 & -\sqrt{2}D \\ -\sqrt{2}D & \tfrac{3}{4}+D \end{pmatrix} \begin{matrix} |j\hat{1}\rangle, \\ |j\hat{0}\ -\rangle, \end{matrix} \tag{33d}$$
$$P_5 = \begin{pmatrix} \tfrac{3}{8}+C/4+\tfrac{3}{4}D & \sqrt{2}C \\ \sqrt{2}C & \tfrac{3}{4}-C \end{pmatrix} \begin{matrix} |j\hat{1}\rangle, \\ |j\hat{0}\ +\rangle. \end{matrix} \tag{33e}$$

Orthogonalization and normalization procedures are described in detail in Ref. 1.

V. CHANGE OF AXIS OF QUANTIZATION

Suppose we know one component of a given representation Γ_i by its decomposition on the base $|jm\rangle_4$ of standard vectors associated to the quaternary axis of quantization 0z. The question is what is its expression on the base $|jm\rangle_3$ of standard vectors associated to the ternary axis of quantization 0Z, and vice versa? Moreover, for any representation of dimension greater than 1, knowing only one component, say in the quaternary axis, we want to derive all components in the ternary axis; this is possible due to the existence of interrelations between components.

Since we need coefficients ${}_3\langle jm'|\Gamma_i\hat{q}\rangle_3$ as functions of coefficients ${}_4\langle jm|\Gamma_i\hat{p}\rangle_4$, we have to perform the rotation defined by matrix (1) on two different spaces, namely the space of base vectors and the space of components of the involved representation. Euler angles of matrix (1) are

$$\alpha=\pi,\quad \beta=\psi=\arccos(1/\sqrt{3}),\quad \gamma=3\pi/4. \tag{34}$$

Base vectors transform according to the classical formula

$$|jm\rangle_4 = \sum_{m'} R^{(j)}_{m'm}\left(\pi, \psi, \frac{3\pi}{4}\right)|jm'\rangle_3. \tag{35}$$

Components of representation Γ_i transform according to

$$|\Gamma_i\,\hat{q}\rangle_3 = \sum_p \hat{R}^{(\Gamma_i)}_{pq}\left(-\frac{3\pi}{4}, -\psi, -\pi\right)|\Gamma_i\,\hat{p}\rangle_4, \tag{36}$$

where $\hat{R}^{(\Gamma_i)}$ coincides with a $R^{(j)}$ whenever Γ_i can be identified with a $\mathscr{D}_j$ (i.e., Γ_1, Γ_4, Γ_6, Γ_8 for $j=0, 1, \frac{1}{2}, \frac{3}{2}$).

Let us write the components of $|\Gamma_i\,\hat{p}\rangle_4$ as

$$|\Gamma_i\,\hat{p}\rangle_4 = \sum_\nu a_{p+4\nu}|j\,p+4\nu\rangle_4, \tag{37}$$

where the sum over ν is extended to positive and negative integers.

Combining (35)–(37), we express $|\Gamma_i\,\hat{q}\rangle_3$ by its coefficients on base vectors $|jm'\rangle_3$; the coefficients for $m' \not\equiv q(3)$ vanish and we can write

$$|\Gamma_i\,\hat{q}\rangle_3 = \sum_{p\mu\nu} (-1)^{\mu+\nu} a_{p+4\nu} \hat{d}^{(\Gamma_i)}_{pq}(-\psi) \times d^{(j)}_{q+3\mu,\,p+4\nu}(\psi)|jq+3\mu\rangle_3. \tag{38}$$

In this formula, the dependency on Euler angles α and γ reduces to the sign $(-1)^{\mu+\nu}$. The symbol $\hat{d}^{(\Gamma_i)}$ coincides with the reduced rotation matrix $d^{(j)}$ when Γ_i can be identified with a $\mathscr{D}_j$; for the other representations, matrices $\hat{d}^{(\Gamma_i)}$ have also real elements:

$$|\Gamma_2\,\hat{0}\rangle_3 = |\Gamma_2\,\hat{2}\rangle_4 \qquad ((1/\sqrt{2})(|3\ 2\rangle_4 - |3\ -2\rangle_4)), \tag{39a}$$

$$\begin{pmatrix} |\Gamma_3\,\hat{1}\rangle_3 \\ |\Gamma_3\ -\hat{1}\rangle_3 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} |\Gamma_3\,\hat{0}\rangle_4 \\ |\Gamma_3\,\hat{2}\rangle_4 \end{pmatrix} \qquad \begin{matrix} (|2\ 0\rangle_4) \\ ((1/\sqrt{2})(|2\ 2\rangle_4 + |2\ -2\rangle_4)), \end{matrix} \tag{39b}$$

$$\begin{pmatrix} |\Gamma_5\,\hat{1}\rangle_3 \\ |\Gamma_5\,\hat{0}\rangle_3 \\ |\Gamma_5\ -\hat{1}\rangle_3 \end{pmatrix} = \frac{1}{\sqrt{3}} \begin{pmatrix} (\sqrt{3}-1)/2 & -1 & (-\sqrt{3}-1) \\ -1 & 1 & -1 \\ (\sqrt{3}+1)/2 & 1 & (-\sqrt{3}+1)/2 \end{pmatrix} \begin{pmatrix} |\Gamma_5\,\hat{1}\rangle_4 \\ |\Gamma_5\,\hat{2}\rangle_4 \\ |\Gamma_5\ -\hat{1}\rangle_4 \end{pmatrix} \qquad \begin{matrix} (-|2\ 1\rangle_4) \\ ((1/\sqrt{2})(|2\ 2\rangle_4 - |2\ -2\rangle_4)), \\ (|2\ -1\rangle_4), \end{matrix} \tag{39c}$$

$$\begin{pmatrix} |\Gamma_7\,\hat{\tfrac{1}{2}}\rangle_3 \\ |\Gamma_7\ -\hat{\tfrac{1}{2}}\rangle_3 \end{pmatrix} = \begin{pmatrix} -\sin(\psi/2) & -\cos(\psi/2) \\ -\cos(\psi/2) & \sin(\psi/2) \end{pmatrix} \begin{pmatrix} |\Gamma_7\,\tfrac{3}{4}\rangle_4 \\ |\Gamma_7\ -\tfrac{3}{2}\rangle_4 \end{pmatrix} \qquad \begin{matrix} (-(\sqrt{5}/\sqrt{6})|\tfrac{5}{2}\ \tfrac{3}{2}\rangle_4 + (1/\sqrt{6})|\tfrac{5}{2}\ -\tfrac{5}{2}\rangle_4), \\ (-(\sqrt{5}/\sqrt{6})|\tfrac{5}{2}\ -\tfrac{3}{2}\rangle_4 + (1/\sqrt{6})|\tfrac{5}{2}\ \tfrac{5}{2}\rangle_4), \end{matrix} \tag{39d}$$

where the basic representations are contained inside parentheses for the quaternary axis and given by formulas (5) and (8) for the ternary axis.

If we know only one quaternary component $|\Gamma_i\,\hat{p}\rangle_4$, formula (38) cannot be used to yield all ternary components $|\Gamma_i\,\hat{q}\rangle_3$ since it involves a sum over p. However, if we rotate only base vectors, i.e., if we combine formulas (35) and (37), the unnormalized ternary components are the restriction of the result to each subspace of D_3; the same result, including normalization information, is obtained without having to worry about α and γ, by multiplying Eq. (38) by the inverse matrix $(\hat{d}^{(\Gamma_i)})^{-1}_{qp}$ and summing over q:

$$|\Gamma_i\,\hat{p}\rangle_4 = \sum_q (\hat{d}^{(\Gamma_i)})^{-1}_{qp} |\Gamma_i\,\hat{q}\rangle_3 = \sum_q \sum_{\mu\nu} d^{(j)}_{q+3\mu,\,p+4\nu}(\psi) a_{p+4\nu} |j\,q+3\mu\rangle_3. \tag{40}$$

The normalized component $|\Gamma_i\,\hat{q}\rangle_3$ is obtained by dividing the associated partial sum in the third member of Eq. (40) by the matrix element $(\hat{d}^{(\Gamma_i)})^{-1}_{qp}$. We should note however that this procedure cannot separate $|\Gamma_8\,\tfrac{3}{2}\rangle$ and $|\Gamma_8\ -\tfrac{3}{2}\rangle$, which are obtained by the appropriate linear combination of formula (40) written for $p = \tfrac{3}{2}$ and $p = -\tfrac{3}{2}$.

As will be shown in Sec. VI, matrix elements $d_{mm'}(\psi)$ for integer values of j have the structure $u + v\sqrt{3}$, where u^2 and v^2 are rational; this leads us to introduce the two matrices $\mathscr{C}$ and $\mathscr{D}$ whose elements are square roots of rational numbers:

$$\mathscr{C}^{(j)}_{m'm} = \frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}} \times \{d^{(j)}_{m'm}(\psi) + (-1)^{m+m'} d^{(j)}_{m'm}(\pi-\psi)\}, \tag{41}$$

$$\mathscr{D}^{(j)}_{m'm} = \frac{1}{\sqrt{(1+\delta_{m0})(1+\delta_{m'0})}} \times \{d^{(j)}_{m'm}(\psi) - (-1)^{m+m'} d^{(j)}_{m'm}(\pi-\psi)\}.$$

These linear combinations appear naturally when we introduce in formula (40) base vectors of subspaces invariant under D_4 and D_3 [formulas (3) and (4) of this paper, and (2) and (3) of paper I; they also appear when adding or subtracting the two equations obtained by writing (40) for p and $-p$ when applicable. For half-integer values of j, we similarly introduce matrices $\mathscr{A}$ and $\mathscr{B}$ whose elements are square roots of rational numbers:

$$\mathscr{A}^{(j)}_{m'm} = \cos\frac{\psi}{2} d^{(j)}_{m'm}(\psi) + (-1)^{m-m'} \times \sin\frac{\psi}{2} d^{(j)}_{m'm}(\pi-\psi),$$

$$\mathscr{B}^{(j)}_{m'm} = \cos\frac{\psi}{2} d^{(j)}_{m'm}(\psi) - (-1)^{m-m'} \times \sin\frac{\psi}{2} d^{(j)}_{m'm}(\pi-\psi). \tag{42}$$

The ternary coefficients are deduced from the quaternary ones, and vice versa, by the two following formulas, which are the consequence of Eq. (40):

$$|\Gamma_i\,\hat{q}\rangle_3 = \sum_{\mu\nu} (-1)^{\mu+\nu} b_{p+4\nu} \mathscr{M}_{p+4\nu,q+3\mu} |j\,q+3\mu\rangle_{D_3},$$

$$|\Gamma_i\,\hat{p}\rangle_4 = \sum_{\mu\nu} (-1)^{\mu+\nu} b_{q+3\mu} \mathscr{M}_{p+4\nu,q+3\mu} |j\,p+4\nu\rangle_{D_4}. \tag{43}$$

In the above expressions, μ and ν are integers, $p+4\nu$ and $q+3\mu$ are labels of base vectors of subspaces of D_4 and D_3, $b_{p+4\nu}$ and $b_{q+3\mu}$ are quaternary and ternary coefficients on these subspaces, and $\mathscr{M}$ is a linear combination of the matrices $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$, $\mathscr{D}$ as indicated in Table III. Note that, in some cases when both components $\hat{p}$ and $-\hat{p}$ exist, two expressions for $\mathscr{M}$ lead to the same result.

TABLE III. Matrices $\mathscr{M}$ of relation (43). When more than one expression is listed, they are equivalent.

i	p	q	$\mathscr{M}$
1	0	0	$\mathscr{C}$
2	2	0	$\mathscr{D}$
3	0	1	$-\mathscr{C}$
		-1	$-\mathscr{C}$
	2	1	$\mathscr{D}$
		-1	$-\mathscr{D}$
4	1	1	$\mathscr{C}, \sqrt{3}\,\mathscr{D}$
		0	$(\sqrt{3}/\sqrt{2})\mathscr{D}$
		-1	$\mathscr{C}, -\sqrt{3}\,\mathscr{D}$
	0	1	$-(\sqrt{3}/\sqrt{2})\mathscr{D}$
		0	$\sqrt{3}\,\mathscr{D}$
		-1	$(\sqrt{3}/\sqrt{2})\mathscr{D}$
	-1	1	$\mathscr{C}, -\sqrt{3}\,\mathscr{D}$
		0	$-(\sqrt{3}/\sqrt{2})\mathscr{D}$
		-1	$\mathscr{C}, \sqrt{3}\,\mathscr{D}$
5	1	1	$-\sqrt{3}\,\mathscr{C}, \mathscr{D}$
		0	$-(\sqrt{3}/\sqrt{2})\mathscr{C}$
		-1	$\sqrt{3}\,\mathscr{C}, \mathscr{D}$
	2	1	$-(\sqrt{3}/\sqrt{2})\mathscr{C}$
		0	$\sqrt{3}\,\mathscr{C}$
		-1	$(\sqrt{3}/\sqrt{2})\mathscr{C}$
	-1	1	$-\sqrt{3}\,\mathscr{C}, -\mathscr{D}$
		0	$-(\sqrt{3}/\sqrt{2})\mathscr{C}$
		-1	$\sqrt{3}\,\mathscr{C}, -\mathscr{D}$
6	$\frac{1}{2}$	$\frac{1}{2}$	$\mathscr{A}, \sqrt{3}\,\mathscr{B}$
		$-\frac{1}{2}$	$(\sqrt{3}/\sqrt{2})\mathscr{B}$
	$-\frac{1}{2}$	$\frac{1}{2}$	$-(\sqrt{3}/\sqrt{2})\mathscr{B}$
		$-\frac{1}{2}$	$\mathscr{A}, \sqrt{3}\,\mathscr{B}$
7	$\frac{3}{2}$	$\frac{1}{2}$	$-(\sqrt{3}/\sqrt{2})\mathscr{A}$
		$-\frac{1}{2}$	$-\sqrt{3}\,\mathscr{A}, -\mathscr{B}$
	$-\frac{3}{2}$	$\frac{1}{2}$	$-\sqrt{3}\,\mathscr{A}, -\mathscr{B}$
		$-\frac{1}{2}$	$(\sqrt{3}/\sqrt{2})\mathscr{A}$
8	$\frac{3}{2}$	$\frac{3}{2}$	$\mathscr{A} + 1/\sqrt{3}\,\mathscr{B}$
		$\frac{1}{2}$	$\sqrt{6}\,\mathscr{A}, \sqrt{2}\,\mathscr{B}$
		$-\frac{1}{2}$	$\sqrt{3}\,\mathscr{A}$
		$-\frac{3}{2}$	$-\sqrt{2}\,\mathscr{A} + (2\sqrt{2}/\sqrt{3})\mathscr{B}$
	$\frac{1}{2}$	$\frac{3}{2}$	$-\sqrt{2}\,\mathscr{B}$
		$\frac{1}{2}$	$\sqrt{3}\,\mathscr{B}$
		$-\frac{1}{2}$	$\sqrt{2}\,\mathscr{A}, \sqrt{6}\,\mathscr{B}$
		$-\frac{3}{2}$	$\sqrt{3}\,\mathscr{A} - \mathscr{B}$
	$-\frac{1}{2}$	$\frac{3}{2}$	$\sqrt{3}\,\mathscr{A} - \mathscr{B}$
		$\frac{1}{2}$	$-\sqrt{2}\,\mathscr{A}, -\sqrt{6}\,\mathscr{B}$
		$-\frac{1}{2}$	$\sqrt{3}\,\mathscr{B}$
		$-\frac{3}{2}$	$\sqrt{2}\,\mathscr{B}$
	$-\frac{3}{2}$	$\frac{3}{2}$	$\sqrt{2}\,\mathscr{A} - (2\sqrt{2}/\sqrt{3})\mathscr{B}$
		$\frac{1}{2}$	$\sqrt{3}\,\mathscr{A}$
		$-\frac{1}{2}$	$-\sqrt{6}\,\mathscr{A}, -\sqrt{2}\,\mathscr{B}$
		$-\frac{3}{2}$	$\mathscr{A} + (1/\sqrt{3})\mathscr{B}$

VI. STRUCTURE OF COEFFICIENTS

Reduced rotation matrix elements are

$$d^{(j)}_{mm'}(\beta) = \sqrt{(j+m)!(j-m)!)(j+m')!(j-m')!}\times\sum_t \frac{(-)^t}{(j+m-t)!t!(j-m'-t)!(t-m+m')!}\times\cos(\beta/2)^{2j+m-m'-2t}\sin(\beta/2)^{2t-m+m'}. \quad (44)$$

In formulas (25) and (32), φ is such that

$$\cos^2(\varphi/2) = \tfrac{2}{3}, \quad \sin^2(\varphi/2) = \tfrac{1}{3}. \quad (45)$$

Therefore $\cos(\varphi/2)d^{(j)}_{m'm}(\varphi)$ and $\sin(\varphi/2)d^{(j)}_{m'm}(\pi-\varphi)$ have a rational quotient and rational diagonal elements for half-integer values of j, and their combinations $A^{(j)}_{m'm}$ and $B^{(j)}_{m'm}$ have the same property.

For integer values of j, $d^{(j)}_{m'm}(\varphi)$ and $d^{j}_{m'm}(\pi-\varphi)$ have a rational quotient and rational diagonal elements, and their combinations $C^{(j)}_{m'm}$ and $D^{(j)}_{m'm}$ have the same property.

As a consequence, every matrix element of a projector (26) or (33) is the product of the square root $\sqrt{(j+m')!(j-m)!/(j+m)!(j-m')!}$ by a large integer, divided by a power of 3 and maybe by 8 (some other factor $\sqrt{2}$ or $\sqrt{3}$ may also appear, see P_4, P_5, P_8). Diagonal elements are rational, for the square root reduces to unity.

In formulas (41) and (42), angle ψ is such that

$$\cos^2\frac{\psi}{2} = \frac{1}{2}\left(1+\frac{1}{\sqrt{3}}\right), \quad \sin^2\frac{\psi}{2} = \frac{1}{2}\left(1-\frac{1}{\sqrt{3}}\right). \quad (46)$$

A similar structure was already encountered for the icosahedral harmonics,[2] with $\sqrt{5}$ instead of $\sqrt{3}$. We conclude that elements of matrices $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$, and $\mathscr{D}$ are square roots of rational numbers.

VII. CONCLUSION

In paper I, we showed that coefficients of representations relative to a quaternary axis can be expressed in a closed form involving only reduced matrix elements of angle $\beta = \pi/2$. For the ternary axis we obtain a similar result with angle $\beta = \varphi = \arccos\frac{1}{3}$. The way to build an orthonormal set in case of degeneracy is the same, and coefficients are square roots of rational numbers. We have given the transformation matrices for going from one system of coefficients to the other, and they equally have the same arithmetic structure.

All representations can be expressed in terms of Γ_1, Γ_2, Γ_3, only, as announced in paper I. This fact is independent of the axis of quantization, but some expressions are different, details will be given in a forthcoming paper which will include tables of Γ_1, Γ_2, Γ_3, up to $j = 25$ in terms of prime factors, for both axes of quantization.

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A nilpotent prolongation of the Robinson–Trautman equation

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(Received 13 February 1984; accepted for publication 15 June 1984)

A prolongation is constructed, in the sense of Wahlquist and Estabrook, for the nonlinear evolution equation determining Robinson–Trautman space-times. The Lie algebra so obtained is found to be (naturally) seven-dimensional and nilpotent. Representations of the algebra are considered. The simple relationship of such a prolongation to the conservation laws associated with the Robinson–Trautman equation is discussed.

PACS numbers: 02.30. – f, 04.20.Jb

I. INTRODUCTION

The prolongation procedure developed by Wahlquist and Estabrook[1] has been used, with some success, to investigate a number of physically interesting nonlinear evolution equations. For example, linear scattering problems and Bäcklund transformations have been associated with nonlinear evolution equations.[2,3]

Useful as the procedure has proven to be, it is as yet, not completely systematic and there is no *a priori* way of knowing if a particular application of it will be successful. As well as attempting to develop general techniques which will enable the method to be carried out as algorithmically as possible,[4] it is useful to produce examples in which various consequences of the prolongation of different equations are explored. It is with the latter aim that we consider in this paper the prolongation of a nonlinear evolution equation that occurs in the study of general relativity.

The successful prolongations of nonlinear evolution equations have usually lead to incomplete Lie algebras of vector fields, which are subject to certain constraints. The constraints are often insufficient for one to be able to deduce (say by repeated application of the Jacobi identities) that the algebra is finite dimensional. Indeed, in important cases such as the Korteweg–deVries (KdV) equation,[5] the algebra is infinite dimensional. Somewhat *ad hoc* procedures are then used to "close off" this algebra, i.e., to find a nontrivial homomorphism of the infinite Lie algebra into a finite-dimensional Lie algebra. It is the representations of the finite-dimensional algebras which have been used in the association of a Bäcklund transformation or linear scattering problem with nonlinear evolution equations. The finite algebras usually dealt with in that context are (semi) simple, but solvable (and nilpotent) algebras also arise and have, to a certain extent, been considered, particularly in relation to nonlocal currents.[5,6]

The equation considered here arises in the study of vacuum solutions of Einstein's gravitational field equations which admit a one-parameter family of shear-free, diverging null hypersurfaces.[7] When such a "Robinson–Trautman" system is axially symmetric, Einstein's equations reduce to a single autonomous nonlinear evolution equation for one dependent variable (z) which is a function of two independent variables (x,t). This equation (the Robinson–Trautman equation) admits an autonomous Wahlquist–Estabrook prolongation in which the Lie algebra is in fact finite dimensional. No "closing off" is needed. The resulting Lie algebra is seven-dimensional and nilpotent. Two representations of this algebra are considered, one nonlinear and the other linear. The nonlinear representation is used to indicate that the existence of the seven-dimensional prolongation is merely a reflection of the fact that the Robinson–Trautman equation admits a finite number of potentials and associated local conservation laws. The conservation laws are local in the sense that the densities and currents do not depend explicitly on the independent variables of the equation. They may, however, depend on the potentials. The linear representation is used to associate a set of linear differential equations with the Robinson–Trautman equation. The linear equations lead to nonlocal conservation laws.

The finite-dimensional nilpotent prolongation obtained here contains little information which cannot be obtained directly from the evolution equation and its related potentials. However, the results suggest that, even if this is generally true, such information may be most efficiently extracted by the use of the prolongation technique.

II. THE EQUATION AND ITS POTENTIALS

For Robinson–Trautman vacuum space-times which are axially symmetric and Petrov type II, local coordinates (t,r,x,ϕ) exist such that the metric can be written in the form[8]

$$ds^2 = (6K - 24r^{-1} + rz^{-1}z_t)dt^2 + 2\,dt\,dr - \tfrac{1}{12}r^2 z(dx^2 + d\phi^2).$$

Here the level surfaces of constant t are shear-free null hypersurfaces, r is an affine parameter along the null geodesics generating these hypersurfaces, and x and ϕ are local coordinates for the two-surfaces given by the intersection of the level sets of t and r. For constant t, $K(z)$ is the Gaussian curvature of the two-surface with metric $\frac{1}{2}z(dx^2 + d\phi^2)$.

The vacuum Einstein field equations reduce to a single equation, the Robinson–Trautman equation, for $z(t,x)$,

$$z_t - K_{xx} = 0, \tag{2.1a}$$

$$K(z) := z^{-3}[(z_x)^2 - zz_{xx}], \tag{2.1b}$$

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where the subscripts denote partial derivatives with respect to t and x. Here, all considerations are local and we do not consider the global conditions which physically valid solutions z must satisfy,[9] but merely assume that all functions are locally as well behaved as is needed. [The Schwarzschild solution corresponds to $z = a_0^2 \cosh^{-2}(x)$, a_0 const.]

It is a straightforward matter to deduce, from Eq. (2.1), a number of conservation laws of the type

$$d\Omega = (T_t + X_x)dt \wedge dx = 0, \tag{2.2a}$$

where the one-form Ω is given by

$$\Omega := T\,dx - X\,dt. \tag{2.2b}$$

Equation (2.2a) is called a "local" conservation law when T and X are not explicitly functions of x and t, and "nonlocal" when T and X also depend on the independent variables t and x.

First, since Eq. (2.1) is of this type, consider the one-form α^1:

$$\alpha^1 := z\,dx + K_x\,dt. \tag{2.3a}$$

Equation (2.1a) is equivalent to $d\alpha^1 = 0$, and so there exists (locally) a potential $p(t,x)$ such that

$$\alpha^1 = dp. \tag{2.3b}$$

p satisfies [from (2.3) and (2.1b)]

$$p_t - [K(p_x)]_x = 0, \tag{2.4}$$

where $p_x = z$. Equation (2.4) is equivalent to $d\alpha^2 = 0$, where

$$\alpha^2 := p\,dx + K(p_x)\,dt, \tag{2.5a}$$

and so there exists a second potential u, such that

$$\alpha^2 = du. \tag{2.5b}$$

Equating (2.5a) and (2.5b) implies that u satisfies

$$u_t - K(u_{xx}) = 0. \tag{2.6}$$

Two further potentials, v and w, can be deduced from (2.1b) combined with (2.4), since it follows from those two equations that

$$[(p)^2]_t - 2[pK + z_x/z]_x = 0, \tag{2.7}$$

and

$$[(p)^3]_t - 3[(p)^2K + 2pz_x/z - 2z]_x = 0. \tag{2.8}$$

Equations (2.7) and (2.8) are equivalent to $d\alpha^3 = 0$ and $d\alpha^4 = 0$, with one-forms α^3 and α^4 defined as

$$\alpha^3 := (p)^2\,dx + 2(pK + z_x/z)dt, \tag{2.9a}$$

$$\alpha^4 := (p)^3\,dx + 3[(p)^2K + 2pz_x/z - 2z]dt. \tag{2.10a}$$

It follows that v and w exist such that

$$\alpha^3 = dv, \tag{2.9b}$$

$$\alpha^4 = dw. \tag{2.10b}$$

It is also straightforward to write down the evolution equations for v and w and they, along with (2.6), may be useful in the search for solutions. They are not, however, needed here. It will be seen in Sec. IV that the functions z, its derivatives, and p, u, v, and w, play a determining role when the prolongation of Eq. (2.1) is considered.

For later reference, note that one can always adjoin a one-form

$$\alpha^5 = c_1\,dx + c_2\,dt, \tag{2.11a}$$

where c_1 and c_2 are constants, so that $d\alpha^5 = 0$ trivially. A potential q exists such that

$$\alpha^5 = dq. \tag{2.11b}$$

III. THE PROLONGATION

The Robinson–Trautman equation (2.1) can be represented by a differential ideal I of two-forms, defined on a subset U of $\mathbb{R}^6$, with local coordinates x, t, z, z_1, z_2, and z_3. The ideal can be generated by the four two-forms

$$\begin{aligned}\beta^1 &= (dz - z_1\,dx)\wedge dt,\\ \beta^2 &= (dz_1 - z_2\,dx)\wedge dt,\\ \beta^3 &= (dz_2 - z_3\,dx)\wedge dt,\\ \beta^4 &= dz\wedge dx + dK_1\wedge dt,\end{aligned} \tag{3.1}$$

where

$$K = z^{-3}[(z_1)^2 - zz_2]$$

and

$$K_1 = -z^{-4}[3(z_1)^3 - 4zz_1z_2 + (z)^2z_3].$$

The ideal is closed, and the generators vanish on a subset V of $\mathbb{R}^2$, with coordinates x and t, when z is a solution of Eq. (2.1). On V

$$z_1 = z_x, \quad z_2 = z_{xx}, \quad z_3 = z_{xxx}, \quad K_1 = K_x.$$

Following Wahlquist and Estabrook, a prolonged ideal $\tilde{I}$ is defined on $U \times \mathbb{R}^n$ with generators $\beta^1, \beta^2, \beta^3, \beta^4$, and the n-vector valued one-form

$$\boldsymbol{\theta} = d\mathbf{y} + \mathbf{F}\,dx + \mathbf{G}\,dt. \tag{3.2}$$

$\mathbb{R}^N$ has coordinates $\mathbf{y} = \{y^A, A = 1,\ldots,n\}$, and $\mathbf{F}$ and $\mathbf{G}$ are n-vector valued functions on $U \times \mathbb{R}^n$. However, since the differential equation is autonomous, we follow the usual procedure of assuming that $\mathbf{F}$ and $\mathbf{G}$ are not functions of x and t. The requirement that the "autonomous" prolonged ideal $\tilde{I}$ be closed under exterior differentiation leads to the following expressions for $\mathbf{F}$ and $\mathbf{G}$:

$$\begin{aligned}\mathbf{F} &= z\mathbf{X}_1 + \mathbf{X}_2,\\ \mathbf{G} &= \ln(z)\mathbf{X}_0 + K_1\mathbf{X}_1 - K\mathbf{X}_3 - (z_1/z)\mathbf{X}_4 + z\mathbf{X}_5 + \tfrac{1}{3}\mathbf{X}_6,\end{aligned} \tag{3.3}$$

where $\mathbf{X}_i$ $(i = 0,1,\ldots,6)$ are vector fields on $\mathbb{R}^n$ alone. $\mathbf{X}_1$, $\mathbf{X}_2$, and $\mathbf{X}_6$ arise as integration "constants" and $\mathbf{X}_0$, $\mathbf{X}_3$, $\mathbf{X}_4$, and $\mathbf{X}_5$ are defined by the vector field Lie brackets

$$\begin{aligned}&[\mathbf{X}_1,\mathbf{X}_2] = :\mathbf{X}_3, \quad [\mathbf{X}_1,\mathbf{X}_3] = :-\mathbf{X}_4,\\ &[\mathbf{X}_2,\mathbf{X}_4] = :-\mathbf{X}_0, \quad [\mathbf{X}_1,\mathbf{X}_4] = :-\mathbf{X}_5.\end{aligned} \tag{3.4a}$$

The commutators which arise directly from the requirement that $\tilde{I}$ be closed are

$$\begin{aligned}&[\mathbf{X}_0,\mathbf{X}_1] = 0, \quad [\mathbf{X}_0,\mathbf{X}_2] = 0,\\ &[\mathbf{X}_2,\mathbf{X}_3] = 0, \quad [\mathbf{X}_2,\mathbf{X}_6] = 0,\\ &[\mathbf{X}_1,\mathbf{X}_5] = 0, \quad [\mathbf{X}_2,\mathbf{X}_5] = -\tfrac{1}{3}[\mathbf{X}_1,\mathbf{X}_6].\end{aligned} \tag{3.4b}$$

It follows immediately from an application of the Jacobi identities to $\mathbf{X}_1,\mathbf{X}_2,\mathbf{X}_3$, and Eq. (3.4) that

$$\mathbf{X}_0 = 0. \tag{3.5}$$

If one further vector field $\mathbf{X}_7$ is defined by

$$\mathbf{X}_7 := -\tfrac{1}{3}[\mathbf{X}_1, \mathbf{X}_6], \tag{3.6}$$

it can be seen directly that $\{\mathbf{X}_1,...,\mathbf{X}_7\}$ generates a seven-dimensional nilpotent Lie algebra with commutator table ($[\mathbf{X}_a, \mathbf{X}_b]$ is in row $\mathbf{X}_a$, column $\mathbf{X}_b$),

	$\mathbf{X}_1$	$\mathbf{X}_2$	$\mathbf{X}_3$	$\mathbf{X}_4$	$\mathbf{X}_5$	$\mathbf{X}_6$	$\mathbf{X}_7$
$\mathbf{X}_1$	0	$\mathbf{X}_3$	$-\mathbf{X}_4$	$-\mathbf{X}_5$	0	$-3\mathbf{X}_7$	0
$\mathbf{X}_2$		0	0	0	$\mathbf{X}_7$	0	0
$\mathbf{X}_3$			0	$\mathbf{X}_7$	0	0	0
$\mathbf{X}_4$				0	0	0	0
$\mathbf{X}_5$					0	0	0
$\mathbf{X}_6$						0	0
$\mathbf{X}_7$							0

(3.7)

The Lie algebra will be denoted by $\mathcal{N}_7$, and its center is $\mathbf{X}_7$. Since no "closing off" or other *ad hoc* technique has been used in these calculations, the autonomous prolongation has now been completely determined. Equations (3.2) and (3.3) can be rewritten in the form

$$\boldsymbol{\theta} = d\mathbf{y} + \omega^a \mathbf{X}_a \quad (a = 1,...,7), \tag{3.8}$$

where

$$\begin{aligned} &\omega^1 = z\,dx + K_1\,dt, \quad \omega^2 = dx, \\ &\omega^3 = -K\,dt, \quad \omega^4 = -(z_1/z)dt, \\ &\omega^5 = z\,dt, \quad \omega^6 = \tfrac{1}{3}\,dt, \\ &\omega^7 = 0. \end{aligned} \tag{3.9}$$

The one-forms ω^a define[3] an $\mathcal{N}_7$-valued connection Γ with curvature which vanishes on V when z is a solution of the Robinson–Trautman equation. In other words, the equation of parallel transport of $\mathbf{y}$, along curves on V,

$$d\mathbf{y} + \omega^a \mathbf{X}_a = 0 \tag{3.10}$$

is integrable if, and only if, Γ is flat.

The explanation for why $\mathbf{X}_7$ does not appear in the prolongation (i.e., $\omega^7 = 0$) is the following: Equation (3.8) constitutes a prolongation of I if, and only if, $d\theta^A$ is contained in $\tilde{I}$. Since $\mathbf{X}_7$ is the center of $\mathcal{N}_7$, and $C^7_{ab}\omega^a \wedge \omega^b = 0$, it follows that

$$d\theta^A = (d\omega^\alpha - \tfrac{1}{2}C^\alpha_{\beta\gamma}\omega^\beta \wedge \omega^\gamma)X^A_\alpha + d\omega^7 X^A_7 \ (\mathrm{mod}\ \theta^A),$$

where $\alpha, \beta, \gamma = 1,...,6$ and the C^e_{ab} are given implicitly in (3.7). Hence, $\tilde{I}$ is closed when $\omega^1,...,\omega^6$ are given by (3.9) if, and only if, $d\omega^7$ is contained in I. Assuming $\omega^7 = f\,dx + g\,dt$, closure implies

$$\omega^7 = b_1\omega^1 + b_2\omega^2 + b_3\omega^6, \tag{3.11}$$

for real constants b_1, b_2, and b_3. However, this is not a generalization of (3.9), since the generators of $\mathcal{N}_7$ admit an automorphism

$$\begin{aligned} &\mathbf{X}_1 \to \mathbf{X}_1 - b_1\mathbf{X}_7, \quad \mathbf{X}_2 \to \mathbf{X}_2 - b_2\mathbf{X}_7, \\ &\mathbf{X}_3 \to \mathbf{X}_3, \quad \mathbf{X}_4 \to \mathbf{X}_4, \\ &\mathbf{X}_5 \to \mathbf{X}_5, \quad \mathbf{X}_6 \to \mathbf{X}_6 - b_3\mathbf{X}_7, \quad \mathbf{X}_7 \to \mathbf{X}_7. \end{aligned}$$

Consider Eq. (3.8) with ω^7 given by (3.11). Under the automorphism this is equivalent to (3.8) with $\omega^7 = 0$. Therefore, it is sufficient to consider only the quotient of $\mathcal{N}_7$ by $\{\mathbf{X}_7\}$ in the following section.

IV. REPRESENTATIONS OF $\mathcal{N}_7$ AND CONSERVATION LAWS

Whenever one finds a set of potentials for a given evolution equation, it is possible to immediately write down a (Wahlquist–Estabrook) prolongation without going through the steps of Sec. III. This fact is illustrated by relating the results of the previous two sections. When z is a solution of Eq. (2.1), the potentials introduced in Sec. II yield the following equations:

$$\begin{aligned} 0 &= dp - z\,dx - K_x\,dt, \\ 0 &= du - p\,dx - K\,dt, \\ 0 &= dv - (p)^2\,dx - 2(pK + z_x/z)dt, \\ 0 &= dw - (p)^3\,dx - 3[(p)^2K + 2pz_x/z - 2z]dt, \\ 0 &= dq - c_1\,dx - c_2\,dt. \end{aligned} \tag{4.1}$$

These can be interpreted as equations of parallel transport for a five-dimensional vector $\mathbf{y}$, where

$$[y^1, y^2, y^3, y^4, y^5] = [p,u,v,w,q].$$

By comparing Eqs. (4.1) with Eqs. (3.10), and using the notation of Eqs. (3.8) and (3.9), one can immediately write down a prolongation with $n = 5$

$$\begin{aligned} \theta^1 &= dy^1 - \omega^1, \\ \theta^2 &= dy^2 - y^1\omega^2 + \omega^3, \\ \theta^3 &= dy^3 - (y^1)^2\omega^2 + 2y^1\omega^3 + 2\omega^4, \\ \theta^4 &= dy^4 - (y^1)^3\omega^2 + 3(y^1)^2\omega^3 + 6y^1\omega^4 + 6\omega^5, \\ \theta^5 &= dy^5 - c_1\omega^2 - 3c_2\omega^6. \end{aligned} \tag{4.2}$$

For z a solution of the Robinson–Trautman equation, Eqs. (4.2) can be pulled back to Eqs. (4.1) on V. By comparing Eq. (4.2) with the general form of (3.8), one can identify the six vector fields (recall $\theta^A = dy^A + \omega^a X^A_a$)

$$\begin{aligned} \mathbf{X}_1 &= -\partial_1, \\ \mathbf{X}_2 &= -y^1\partial_2 - (y^1)^2\partial_3 - (y^1)^3\partial_4 - c_1\partial_5, \\ \mathbf{X}_3 &= \partial_2 + 2y^1\partial_3 + 3(y^1)^2\partial_4, \\ \mathbf{X}_4 &= 2\partial_3 + 6y^1\partial_4, \\ \mathbf{X}_5 &= 6\partial_4, \\ \mathbf{X}_6 &= -3c_2\partial_5, \end{aligned} \tag{4.3}$$

where $\partial_A := \partial/\partial y^A$, $A = 1,...,5$. These vector fields realize the six-dimensional nilpotent Lie algebra $\mathcal{N}_6$ corresponding to the quotient of $\mathcal{N}_7$ by its center [i.e, obtained from the commutator table (3.7) by formally setting $\mathbf{X}_7 = 0$].

On the other hand, starting from the complete autonomous prolongation obtained in Sec. III, and representing the Lie algebra generators $\mathbf{X}_1,...,\mathbf{X}_6$ by the vector fields on $\mathbb{R}^5$ given by Eq. (4.3) and the center $\mathbf{X}_7$ by the zero vector field, one obtains Eq. (4.1) again.

By way of contrast, consider an evolution equation with an infinite number of potentials (or Wahlquist–Estabrook

pseudopotentials) and conservation laws, such as the KdV equation. The prolongation structure of the KdV equation yields an infinite-dimensional Lie algebra. By imposing an *ad hoc* linear relationship upon certain generators, homomorphisms to finite-dimensional Lie algebras can be obtained. Here, the direct relationship between the potentials of Sec. II and the generators of $\mathcal{N}_7$ suggests that the autonomous prolongation has little more to offer directly than do the potentials themselves.

Many different realizations of $\mathcal{N}_6$ or $\mathcal{N}_7$ can be obtained, of course. Higher-dimensional realizations will result in more potentials. The significance of these is determined from Eqs. (3.10). For example, a faithful six-dimensional realization of $\mathcal{N}_6$ is given by $\mathbf{X}_1$, $\mathbf{X}_3$, $\mathbf{X}_4$, $\mathbf{X}_5$, of Eq. (4.3), with $\mathbf{X}_2$ and $\mathbf{X}_6$ replaced by

$$\mathbf{X}_2 \to \mathbf{X}_2 + (c_1 + y^5)\partial_5, \quad \mathbf{X}_6 \to y^6\partial_6.$$

For this example, it is easily seen from Eqs. (3.10) that, on V, y^5 and y^6 are simple functions of x and t, respectively. In general, the addition of identically conserved quantities to Eqs. (3.10) gives no further information about these equations.

Here, we confine ourselves to the consideration of a linear representation of $\mathcal{N}_7$ in order to associate, in the usual way, a linear system with the Robinson–Trautman equation.

Such a representation of $\mathcal{N}_7$ is given by the following vector fields on $\mathbb{R}^7$:

$$\begin{aligned}
\mathbf{X}_1 &= -y^2\partial_3 + y^3\partial_4 + y^4\partial_5 + 3y^6\partial_7,\\
\mathbf{X}_2 &= y^1\partial_3 - y^5\partial_7,\\
\mathbf{X}_3 &= -y^1\partial_4 - y^4\partial_7,\\
\mathbf{X}_4 &= -y^1\partial_5 + y^3\partial_7,\\
\mathbf{X}_5 &= y^2\partial_7,\\
\mathbf{X}_6 &= -3y^1\partial_7,\\
\mathbf{X}_7 &= 0.
\end{aligned} \tag{4.4}$$

From Eqs. (3.9) and (3.10), (4.4) yields the linear differential equations[10]

$$\frac{\partial}{\partial x}\begin{bmatrix} y^1\\ y^2\\ y^3\\ y^4\\ y^5\\ y^6\\ y^7 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ -1 & z & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & -z & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -z & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 1 & -3z & 0 \end{bmatrix}\begin{bmatrix} y^1\\ y^2\\ y^3\\ y^4\\ y^5\\ y^6\\ y^7 \end{bmatrix}, \tag{4.5}$$

$$\frac{\partial}{\partial t}\begin{bmatrix} y^1\\ y^2\\ y^3\\ y^4\\ y^5\\ y^6\\ y^7 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & K_x & 0 & 0 & 0 & 0 & 0\\ -K & 0 & -K_x & 0 & 0 & 0 & 0\\ -z_x/z & 0 & 0 & -K_x & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 1 & -z & z_x/z & -K & 0 & -3K_x & 0 \end{bmatrix}\begin{bmatrix} y^1\\ y^2\\ y^3\\ y^4\\ y^5\\ y^6\\ y^7 \end{bmatrix}.$$

In this particular case, the effect of choosing a different representation of the Lie algebra in the prolongation can be illustrated by using these equations in a more direct manner than is usually possible. When z is a solution of the Robinson–Trautman equation, it follows in a simple way from Eq. (4.5) that

$$\begin{aligned}
y^1 &= a_1,\\
y^2 &= a_2,\\
y^3 &= a_2 p - a_1 x,\\
y^4 &= a_1(xp - u) - \tfrac{1}{2}a_2(p)^2,\\
y^5 &= \tfrac{1}{2}a_1[2up - x(p)^2 - v] + \tfrac{1}{6}a_2(p)^3,\\
y^6 &= a_3,\\
y^7 &= \tfrac{1}{2}a_1[2t + (u)^2 - xv] + \tfrac{1}{6}a_2 w - 3a_3 p,
\end{aligned} \tag{4.6}$$

where a_1, a_2, and a_3 are constants and p, u, v, and w are the potentials considered previously. Because the functions $y^1,\ldots,y^7$ can be expressed in terms of the potentials in this way, it is possible to rewrite the integrability conditions for the linear system (4.5) explicitly as conservation laws for the Robinson–Trautman and potential equations of Sec. II. These conservation laws are obtained by inserting the functions $\{y^4\}$ from Eq. (4.6) into the integrability conditions

$$(zy^2 - y^1)_t = (y^2K_x)_x, \tag{4.7a}$$

$$(zy^3)_t = (y^1K + y^3K_x)_x, \tag{4.7b}$$

$$(zy^4)_t = (y^1z_x/z + y^4K_x)_x, \tag{4.7c}$$

$$(y^5 - 3zy^6)_t = (y^1 - zy^2 + y^3z_x/z - Ky^4 - 3y^6K_x)_x. \tag{4.7d}$$

Contained in these equations are local and nonlocal conser-

vation laws including the simple, but nonlocal, law for Eq. (2.1) given by [choose $a_1 = -1$, $a_2 = 0$ in (4.7b)]

$$(xz)_t = (-K + xK_x)_x.$$

Such results are not contained in the earlier considerations.

Conclusions regarding the physical significance of the conservation laws obtained here, and exact solutions obtained from the potential equations, will appear elsewhere.

ACKNOWLEDGMENTS

One author (E. G.) is thankful to R. J. McKellar for informative conversations regarding Lie algebras.

Work was supported in part by a Natural Sciences and Engineering Research Council of Canada grant.

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Factorization method and new potentials with the oscillator spectrum

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(Received 2 March 1984; accepted for publication 15 June 1984)

A one-parameter family of potentials in one dimension is constructed with the energy spectrum coinciding with that of the harmonic oscillator. This is a new derivation of a class of potentials previously obtained by Abraham and Moses with the help of the Gelfand–Levitan formalism.

PACS numbers: 02.30.Em, 03.65. – w

I. INTRODUCTION

Contrasted with general relativity, where new solutions are found every now and then, the class of exactly soluble problems of quantum mechanics (QM) has not greatly expanded. The two most commonly used exact methods to determine the spectra in QM are the method of the orthogonal polynomials and the algebraic method of "factorization." The potentials for which exact solutions exist form a rather narrow family, including the elastic and Coulomb potentials (modified by the $1/r^2$ terms), the Morse potential, the square potential wells, and a few others, and the common opinion is that this is everything exactly soluble in Schrödinger's quantum mechanics. Hence, it might be of interest to notice that in some occasions the "factorization" method seems not yet completely explored. In particular, it allows the construction of a class of potentials in one dimension, which have the oscillator spectrum, but which are different from the potential of the harmonic oscillator. This class has been previously derived using the Gelfand–Levitan formalism.

II. CLASSICAL FACTORIZATION METHOD

The factorization method in its most classical form was first used to determine the spectrum of the Hamiltonian of the harmonic oscillator in one dimension:

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2. \tag{2.1}$$

The method consisted of introducing the operators of "creation" and "annihilation"

$$a = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + x\right) = \frac{1}{\sqrt{2}}e^{-x^2/2}\frac{d}{dx}e^{x^2/2}, \tag{2.2}$$

$$a^* = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + x\right) = -\frac{1}{\sqrt{2}}e^{x^2/2}\frac{d}{dx}e^{-x^2/2}, \tag{2.3}$$

with the properties

$$\left.\begin{aligned} a^*a &= H - \tfrac{1}{2} \\ aa^* &= H + \tfrac{1}{2} \end{aligned}\right\} \Rightarrow [a, a^*] = 1. \tag{2.4}$$

Hence,

$$Ha^* = a^*(H + 1), \tag{2.5}$$

$$Ha = a(H - 1). \tag{2.6}$$

These relations allow the construction of the eigenvectors and eigenvalues of H. If ψ is an eigenvector of H ($H\psi = \lambda\psi$) the functions $a^*\psi$ and $a\psi$ [provided that they are nonzero and belong to $L^2(R)$] are new eigenvectors corresponding to the eigenvalues $\lambda + 1$ and $\lambda - 1$, respectively:

$$H(a^*\psi) = a^*(H + 1)\psi = (\lambda + 1)a^*\psi, \tag{2.7}$$

$$H(a\psi) = a(H - 1)\psi = (\lambda - 1)a\psi. \tag{2.8}$$

Since the operator H is positively definite, one immediately finds the lowest energy eigenstate ψ_0 as the one for which

$$a\psi_0 = 0 \Rightarrow \frac{d}{dx}e^{x^2/2}\psi_0 = 0 \Rightarrow \psi_0(x) = C_0 e^{-x^2/2}, \tag{2.9}$$

and one checks that the corresponding eigenvalue is $\lambda_0 = \frac{1}{2}$. Using now the operator a^*, one subsequently constructs the ladder of other eigenvectors ψ_n corresponding to the next eigenvalues $\lambda_n = n + \frac{1}{2}$:

$$\psi_n = C_n(a^*)^n\psi_0 = C_n(-1)^n\left[e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}\right]e^{-x^2/2}$$

$$= C_n H_n(x)e^{-x^2/2}, \tag{2.10}$$

where $H_n(x)$ are the Hermite polynomials given by the Rodriguez formula

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}. \tag{2.11}$$

The nonexistence of any other spectrum points and eigenstates follows from the completeness of the Hermite polynomials. The above method was first employed by Dirac.[1] Its extension for the hydrogen atom was found by Infeld and Hull.[2] A generalized presentation is due to Plebañski.[3] The group theoretical meaning is owed to Moshinsky,[4] Wolf,[5] and other authors. Yet, there is still one aspect of the method relatively unexplored. It can be used not only to find the interdependence between different spectral subspaces of the same operator but also to transform one Hamiltonian into another.

III. MODIFIED HAMILTONIAN

Consider once more the factorized expression

$$H + \tfrac{1}{2} = aa^*. \tag{3.1}$$

Are the operators a and a^* here unique? Define the new operators

$$b = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + \beta(x)\right), \tag{3.2}$$

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$$b^* = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + \beta(x)\right), \tag{3.3}$$

and demand that $H + \frac{1}{2}$ be written alternatively as

$$H + \tfrac{1}{2} = bb^*. \tag{3.4}$$

This leads to

$$-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \frac{1}{2} = \frac{1}{2}\left(-\frac{d^2}{dx^2} + \beta' + \beta^2\right), \tag{3.5}$$

and so, the condition for β is the Ricatti equation

$$\beta' + \beta^2 = 1 + x^2. \tag{3.6}$$

The occurrence of the Ricatti equation in the factorization problems is a typical phenomenon.[2,3] In general, the explicit solution of this type of equation is not known. This is not the case in (3.6), where one has one particular solution $\beta = x$. Hence, the general solution can be obtained putting $\beta = x + \phi(x)$. This yields

$$\phi' + 2\phi x + \phi^2 = 0 \rightarrow \phi'/\phi^2 + 2x(1/\phi) + 1 = 0. \tag{3.7}$$

Introducing now a new function $y = 1/\phi$, one ends up with a first-order linear inhomogeneous equation

$$-y' + 2xy + 1 = 0, \tag{3.8}$$

whose general solution is

$$y = \left(\gamma + \int_0^x e^{-x'^2}dx'\right)e^{x^2}, \quad \gamma \in R.$$

Hence,

$$\phi(x) = \frac{e^{-x^2}}{\gamma + \int_0^x e^{-x'^2}dx'} \Rightarrow \beta(x) = x + \frac{e^{-x^2}}{\gamma + \int_0^x e^{-x'^2}dx'}. \tag{3.9}$$

The introduction of the operators b, b^* might seem to offer little new, as we have still $bb^* = aa^* = H + \frac{1}{2}$. However, the commutator of b and b^* is not a number:

$$[b, b^*] = \beta'(x) = 1 + \phi'(x). \tag{3.10}$$

Hence, the inverted product b^*b is not H + const, but it defines a certain new Hamiltonian

$$b^*b = bb^* + [b^*, b] = H + \tfrac{1}{2} - 1 - \phi' = H' - \tfrac{1}{2}, \tag{3.11}$$

where

$$H' = H - \phi'(x) = -\frac{1}{2}\frac{d^2}{dx^2} + V(x), \tag{3.12}$$

with

$$V(x) = \frac{x^2}{2} - \frac{d}{dx}\left[\frac{e^{-x^2}}{\gamma + \int_0^x e^{-x'^2}dx'}\right]. \tag{3.13}$$

If $|\gamma| > \frac{1}{2}\sqrt{\pi}$, the above potential has no singularity and behaves like $x^2/2$ for $x \rightarrow \pm\infty$; and so, one obtains here a one-parameter family of self-adjoint Hamiltonians in $L^2(R)$. As one can immediately see, their spectra are identical to that of the harmonic oscillator, though their eigenvectors are different. Indeed, (3.4) and (3.11) imply

$$H'b^* = (b^*b + \tfrac{1}{2})b^* = b^*(bb^* + \tfrac{1}{2}) = b^*(H + 1). \tag{3.14}$$

Hence, for ψ_n $(n = 0, 1, ...)$ being the eigenvectors of H, the functions

$$\phi_1 = b^*\psi_0, \quad \phi_2 = b^*\psi_1, ..., \quad \phi_n = b^*\psi_{n-1}, ... \tag{3.15}$$

are the eigenvectors of H' corresponding to the same eigenvalues $\lambda_n = n + \frac{1}{2}$:

$$H'\phi_n = H'b^*\psi_{n-1} = b^*(H + 1)\psi_{n-1} = b^*(n + \tfrac{1}{2})\psi_{n-1}$$
$$= (n + \tfrac{1}{2})\phi_n \quad (n = 1, 2, ...). \tag{3.16}$$

The functions ϕ_n are square integrable because of the asymptotic behavior of $\phi(x)$ for $x \rightarrow \pm\infty$. They are obviously orthogonal, as $(\phi_j, \phi_k) = (b^*\psi_{j-1}, b^*\psi_{k-1}) = (\psi_{j-1}, bb^*\psi_{k-1}) = (\psi_{j-1}, (H + \frac{1}{2})\psi_{k-1}) = k(\psi_{j-1}, \psi_{k-1}) = 0$, for $k \neq j$. However, they do not yet span the whole of $L^2(R)$. The missing element is the vector ϕ_0 orthogonal to all of ϕ_n $(n = 1, 2, ...)$,

$$(\phi_0, \phi_n) = (\phi_0, b^*\psi_{n-1}) = 0 \Rightarrow (b\phi_0, \psi_{n-1}) = 0$$
$$(\text{for } n = 1, 2, ...) \Rightarrow b\phi_0 = 0, \tag{3.17}$$

and so, the "missing vector" is found from the first-order differential equation

$$b\phi_0 = \frac{1}{\sqrt{2}}\left[\frac{d}{dx} + \beta(x)\right]\phi_0 = 0$$
$$\Rightarrow \phi_0 = c_0 e^{-x^2/2}\exp\left(\int_0^x \phi(x')dx\right). \tag{3.18}$$

By the very definition (3.18), ϕ_0 is another eigenvector of H' corresponding to the eigenvalue $\lambda_0 = \frac{1}{2}$:

$$H'\phi_0 = (b^*b + \tfrac{1}{2})\phi_0 = \tfrac{1}{2}\phi_0. \tag{3.19}$$

As the system of vectors $\phi_0, \phi_1, ...$ is complete in $L^2(R)$, the operator (3.12) is a new Hamiltonian, whose spectrum is that of the harmonic oscillator, although the potential is not. Since our initial Hamiltonian is parity invariant, the final conclusion should remain valid when $x \rightarrow -x$. Indeed, though each one of the potentials (3.13) is not parity invariant, the whole class is: $V(-x, \gamma) = V(x, -\gamma)$ $(|\gamma| > \frac{1}{2}\sqrt{\pi})$. The reader can verify that what we have obtained here is the same class of potentials that Abraham and Moses obtained by using the Gelfand–Levitan formalism (Ref. 6, Sec. III, starting on the top of p. 1336; see also papers by Nieto and Gutschick[7] and Nieto[8]).

Remark: Differently than for the oscillator, the eigenvectors ϕ_n admit no first-order differential "rising operator." The ϕ_n's are constructed not by a rising operation, but due to their relation to the ψ_n's, which can be schematically represented as in Fig. 1. This means, however, that for the ϕ_n's there is a differential "rising operator," but it is of the third order: $A^* = b^*a^*b$. As far as we know, the use of the higher-order rising and lowering operators in spectral problems has not yet been explored.

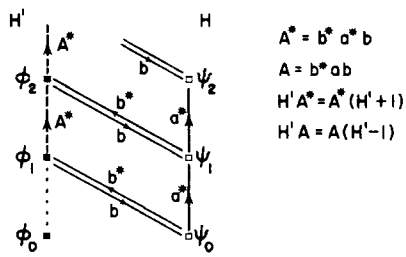

FIG. 1. The relation between the ϕ_n's and the ϕ_n's.

ACKNOWLEDGMENTS

The author is grateful to Augusto García for his kind hospitality at the Departamento de Física del Centro de Investigación y de Estudios Avanzados in México. Thanks are due to Jerzy Plebañski and other colleagues at the Departamento de Física for their interest in this work and helpful discussions. The discussion with Marcos Moshinsky in Oaxtepec in 1982 is remembered.

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The double cnoidal wave of the Korteweg–de Vries equation: An overview

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(Received 22 March 1984; accepted for publication 22 June 1984)

Earlier work of the author on the spatially periodic solutions of the Korteweg–de Vries equation is here extended via an in-depth treatment of a special case. The double cnoidal wave is the simplest generalization of the ordinary cnoidal wave discovered by Korteweg and de Vries in 1895. In the limit of small amplitude, the double cnoidal wave is the sum of two noninteracting linear sine waves. In the oppositie limit of large amplitude, it is the sum of solitary waves of two different heights repeated periodically over all space. Although special, the double cnoidal wave is important because it is but the particular case $N = 2$ of a broad family of solutions known variously as "N-polycnoidal waves," "finite gap," "finite zone" solutions, "waves on a circle," or "N-phase wave trains." It has been shown by others that the set of N-polycnoidal waves gives the general initial value solution to the Korteweg–de Vries equation. This present work is the core of a three-part treatment of the double cnoidal wave. This part, the overview, presents graphic examples in all the important parameter regimes, explains how collision phase shifts alter the average speed of the two wave phases from the "free" velocities of the two solitary waves, describes the different branches or modes of the double cnoidal wave (it is possible to have many solitary waves on each spatial period provided they are of only two distinct sizes), and contrasts the results of this work with the very limited numerical calculations of previous authors. The second part describes how the problem of numerically calculating the double cnoidal wave can be reduced down to solving four algebraic equations by perturbation theory. The third part explains how the so-called "modular transformation" of the Riemann theta functions is important in interpreting N-polycnoidal waves.

PACS numbers: 02.30.Jr, 02.60.Lj

I. INTRODUCTION

The "Hill's spectrum method," developed in the mid-1970's by Lax, Novikov, McKean, and others, has been a powerful theoretical tool for understanding the spatially periodic solutions of the Korteweg–de Vries and other soliton equations. In particular, it showed that there existed solutions which generalize the simple cnoidal waves found by Korteweg and de Vries themselves in 1895. These generalizations were dubbed "polycnoidal waves" in Ref. 1 but they are known alternatively as "finite band" or "finite gap" solutions in the Russian literature and sometimes as "N-phase wave trains" in the American journals. The N-polycnoidal wave is a function of N "phase" variables of the form

$$\zeta_i = k_i(x - c_i t) + \phi_i, \tag{1.1}$$

where the k_i are wavenumbers, the c_i are phase speeds, and the ϕ_i are constant phase factors. The most compact expression for $u(x,t)$ is in terms of a N-dimensional Riemann theta function whose arguments are the N "phase" variables defined in (1.1). Although the polycnoidal waves, like the ordinary cnoidal wave which is the special case $N = 1$, are thus special solutions, it has been shown that the class of polycnoidal waves is dense on the set of solutions of the Korteweg–de Vries (KdV) equation which are spatially periodic. To put it another way, the solution to the KdV equation for an arbitrary initial condition can be approximated for an arbitrary finite time interval to an arbitrary degree of accuracy by an N-polycnoidal wave of appropriate parameters and sufficiently large N. Thus, to understand these special solutions is to understand the general solution, too, at least for finite time.

Unfortunately, like its counterpart, the inverse scattering method for a spatially unbounded domain, the Hill's spectrum method is very complicated and a poor tool for actual numerical calculations. To quote Ferguson *et al.*,[2] "the exact formulas seem to be of little practical use." An alternative approach was discovered by Hirota[3,4] and subsequently generalized to the spatially periodic problem independently by Nakamura[5] and Boyd.[1] The reason for the alternative's effectiveness is that the theta functions satisfy not the KdV equation itself, but rather Hirota's transformed version, which will be called the "Hirota–Korteweg–de Vries" or "HKdV" equation; the solution of the KdV equation is obtained by taking the second derivative with respect to x of the logarithm of the theta function. Because the theta function depends on only a finite number of parameters, it is possible to reduce the problem down to that of solving a finite set of algebraic equations to determine these theta function parameters.

The aim of this paper, which is a sequel to Ref. 1, is to exploit this Hirota-theta function approach to deepen our understanding of the spatially periodic solutions of the Korteweg–de Vries equation, paying particular attention to $N = 2$, the double cnoidal wave. This article and its two companion papers,[6,7] are a single connected work. The other two papers discuss a perturbative (and numerical) solution of the implicit dispersion relation for the theta function parameters and the role of the "special" modular transformation of the theta functions in physically interpreting the polycnoidal wave solutions. This paper will strive to provide a general overview of the physics and mathematics of polycnoidal waves, leaving the technical details to the other two articles

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wherever possible.

Before giving an outline of this work, it is useful to compare and contrast its aims with those of three other schools of polycnoidal wave studies. A. Nakamura and his collaborators R. Hirota, M. Ito, and Y. Matsuno[5,8–10] have developed the direct theta function method by showing, via a mixture of clever theorems and occasional numerical calculations, that it can be used in principle to reduce a large number of different soliton-admitting partial differential equations to a finite set of algebraic equations for the theta function parameters. Equations whose Hirota-transformed equivalent is a set of coupled bilinear equations or a complex equation are discussed as well as the simpler case of those which, like the Korteweg–de Vries equation, transform into a single bilinear equation with real coefficients. They emphasize that a number of as yet unresolved technical difficulties exist for these other classes of equations, which is why this present article is focused specifically on the KdV equation. The limitations of their work are a lack of explicit calculations (except for ordinary cnoidal waves and some numerical computations described in Sec. VII), omission of perturbation theory such as is given in Ref. 6, and restriction to theta Fourier series only. The alternative Gaussian series for the theta function, introduced in Ref. 1, is a better way to explore the near-solitary wave regime.

Forest, McLaughlin, Flaschka, and Ferguson[2,11] have, like the author, attempted to explore polycnoidal waves in the spirit of applied mathematics rather than pure mathematics by taking a "concrete viewpoint," to borrow a phrase from the title of Ferguson *et al.*[2] Though the philosophy thus is similar, the line of attack is very different: this work and Refs. 1, 6, and 7 scrupulously avoid any explicit use of the Hill's spectrum method while Ferguson *et al.*[2] have "Spectral theory" as the first words of their title. Their whole approach is oriented toward understanding polycnoidal waves via calculation of the spectrum of Hill's equation and they avoid all mention of Hirota's transformed bilinear equations, perturbation theory, the special modular transformation, and most of the other topics we will discuss. Thus, their work is complementary to what will be presented here.

The Polish school of Zagrodziński and Jaworski[12] has written an interesting series of papers on the sine-Gordon equation. Their approach is inverse to that used here in that they completey specify the theta matrix and then solve for the wavenumbers k_j. This simplifies much of the analysis at the expense of obtaining generally nonintegral k_j so that their solutions are "almost periodic" rather than periodic in space.

II. AN OVERVIEW OF THE DOUBLE CNOIDAL WAVE

The Hill's spectrum method has shown that the N-polycnoidal wave is most easily expressed in terms of an N-dimensional Riemann theta function via

$$u(x,t) = 12\frac{d^2}{dx^2}\ln[\theta(x,t)], \tag{2.1}$$

where $\theta(x,t)$ is the N-dimensional Riemann theta function and where $u(x,t)$ is the actual solution of the Korteweg–de Vries equation

$$u_t + uu_x + u_{xxx} = 0. \tag{2.2}$$

For the special case $N = 2$, which will be henceforth called the "double cnoidal wave," the theta function is defined by

$$\theta = \sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\exp(-\{T_{11}n_1^2 + 2T_{12}n_1n_2 + T_{22}n_2^2\}) \times\exp[2\pi i(n_1X + n_2Y)], \tag{2.3}$$

where the T_{ij} are the elements of a 2×2 positive definite symmetric matrix known as the "theta matrix" and where X and Y are the "phase variables" defined, as in (1.1), by

$$X = k_1(x - c_1t) + \phi_1, \tag{2.4}$$

$$Y = k_2(x - c_2t) + \phi_2. \tag{2.5}$$

Mathematicians normally define the theta function in terms of an imaginary theta matrix as explained in Appendix A, but the real-valued T_{ij} employed in (2.3) are more convenient for calculations. The independent parameters are the wavenumbers k_1 and k_2, and the diagonal theta matrix elements T_{11} and T_{22}. The dependent parameters are the phase speeds c_1 and c_2, plus the diagonal theta matrix element T_{12}. [There is a fourth dependent parameter, the constant of integration A in the "Hirota–Korteweg–de Vries equation" described in Ref. 6, but this is only a calculational tool and does not appear in the final answer (2.1).]

The wavenumbers k_1 and k_2 can be arbitrary; Novikov[13] has emphasized from his earliest papers that if the wavenumbers are incommensurable, i.e., if k_1/k_2 is an irrational number, then the double cnoidal will be "almost periodic" in space rather than strictly periodic, but this is mathematically legitimate. Although some applications of "spatial almost periodicity" can be envisaged,[14] it is sufficient for most physical problems to take $k_1 = 1$ and $k_2 = 2$. The reasons are that (i) in most Fourier series, the second harmonic ($k = 2$) is the largest component after the fundamental ($k = 1$), and (ii) one can change the spatial period from unity [as in (2.3) with $k_1 = 1$] to an arbitrary period through a trivial rescaling of the coordinates. The spatial period is equal to one in all the figures and cases described in the rest of this paper.

The diagonal theta matrix elements are thus the more important parameters because they specify the amplitude of the two waves that make up the double cnoidal wave. Figure 1 indicates the different wave regimes of the $T_{11} - T_{22}$ plane. When T_{11} and T_{22} are both large, the double cnoidal wave is approximately equal to the sum of two linear, noninteracting sine waves of different wavenumbers and phase speeds, i.e.,

$$u(x,t) = -48\pi^2[k_1^2e^{-T_{11}}\cos(2\pi X) + k_2^2e^{-T_{22}}\cos(2\pi Y)]. \tag{2.6}$$

When both T_{11} and T_{22} are small, the double cnoidal wave is approximately given by the usual Korteweg–de Vries double solitary wave with one tall soliton and one short soliton on each unit interval in x. The Fourier series (2.3) converges very slowly for small T_{11} and T_{22}. The central theme of the author's previous paper[1] is that one should substitute instead the series

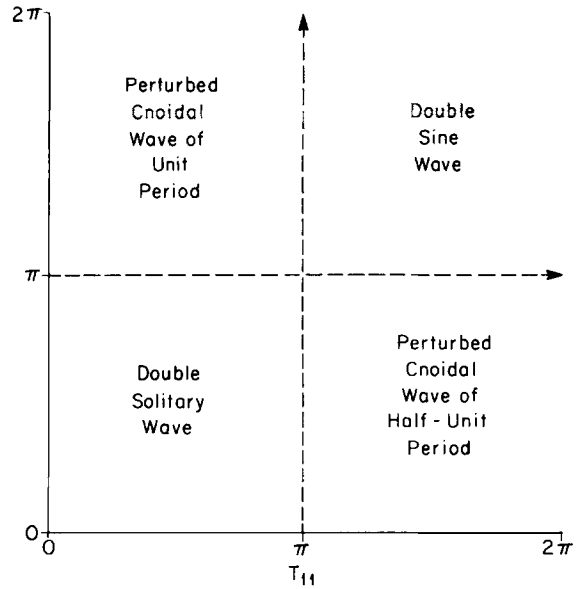

FIG. 1. Schematic diagram showing the four main regimes of the double cnoidal wave in $T_{11} - T_{22}$ plane, where T_{11} and T_{22} are the diagonal theta matrix elements, which are always positive.

$$\theta = \sum_{\substack{n_1=-\infty \\ [\text{half-integers}]}}^{\infty} \sum_{n_2=-\infty}^{\infty} \exp\left(-\left\{ \left(\frac{R_{11}}{2}\right)(X+n_1)^2 + R_{12}(X+n_1)(Y+n_2) + \left(\frac{R_{22}}{2}\right)(Y+n_2)^2 \right\} \right), \tag{2.7}$$

where the sums are over the half-integers, $\pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots$, and where the R_{ij} are proportional to the elements of the inverse of theta matrix formed by the T_{ij}. For obvious reasons, (2.7) will be referred to as the "Gaussian" series of the theta function since each term is a Gaussian function of X and Y; this series is the Poisson sum of the Fourier series. As explained in Appendix B of Ref. 6, the usual double solitary wave can be obtained from (2.7) by truncating it to four terms and taking the second logarithmic derivative as in (2.1), but the result is too messy to repeat here.

The strength of using two alternative series representaions, (2.3) and (2.7), is that the Fourier series converges rapidly in the double sine wave regime where (2.7) converges slowly, while the Gaussian series converges rapidly in the double soliton regime where the Fourier series is almost useless. Consequently, in this paper and its two companions, we shall move from Fourier series to Gaussian series and back again with great freedom. As explained in Ref. 6, the mechanics of calculating the unknown phase speeds and diagonal theta matrix element (either T_{12} or R_{12}) are such that the Fourier-based computation is merely a special case of that for the Gaussian series.

Unfortunately, neither series is rapidly convergent along the T_{11} and T_{22} axes where one diagonal theta matrix element is large in comparison to the other, but this is not of vital importance because these near-axis regimes represent a single solitary wave perturbed by a very small amplitude sine wave. As such, these regimes are much less interesting than those in which the two waves are of equal amplitude since theories for the single soliton subject to an arbitrary perturbation have been developed by R. Grimshaw[15] and others he references. In practice, there is actually a high degree of overlap between the Fourier and Gaussian series both with each other and with the perturbed one-soliton regimes, so the need for special methods for these near-axis double cnoidal waves is usually academic.

The double solitary wave regime is the most interesting case of all. In Sec. IV, the geometry of the X-Y plane is deduced from the Gaussian series. To some extent, this will merely repeat the construction given in Ref. 1 for the single cnoidal wave, but it will also bring out several features such as phase shifts and the special modular transformation which are unique to polycnoidal waves with $N \geqslant 2$, and have no counterpart for the ordinary $N = 1$ cnoidal wave. First, however, some sample graphs are presented to give the reader a feeling for each of the four regimes of the double cnoidal wave.

III. SAMPLE DOUBLE CNOIDAL WAVES

Figures 2–5 illustrate $u(x,t)$ for each of the wave regimes indicated schematically in Fig. 1. The graphs were computed in a frame of reference moving at the phase velocity c_1 so that the tallest peak is approximately stationary; in this frame of reference, the double cnoidal wave is simply periodic in time, so it suffices to show half of one temporal period. Strictly speaking, the double cnoidal wave solution has a mean value of 0, i.e., the integral of $u(x,t)$ over a period is 0, but for visual clarity, a constant[16] has been added to the graphs.

The first case is that of a classic double solitary wave: The tall soliton overtakes the short soliton and only a single peak is visible at the time of maximum interaction. In time, however, the two separate and emerge unchanged by their interaction except for a shift of phase. In other words, the tall peak is briefly accelerated and the short peak briefly deaccelerated by their encounter so that the tall soliton is farther to the right than it would have been in the absence of the collision. In a spatially unbounded domain, where there are just the two solitons on the whole interval $x \in [-\infty, \infty]$, this col-

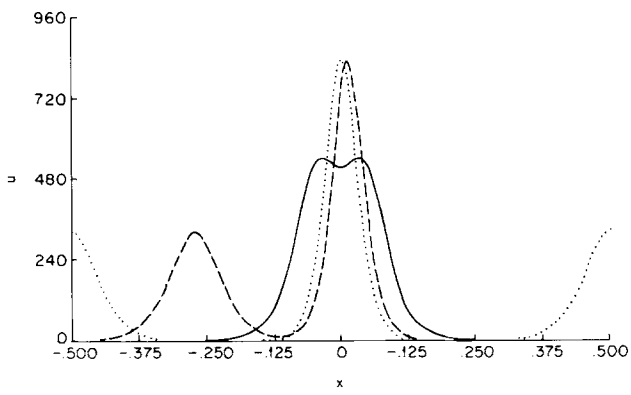

FIG. 2. A Korteweg–de Vries double cnoidal wave in the double soliton regime. The mode in this and the next three figures is $[1,2]^P$ or equivalently, $\{1,1\}^P$, in the notation defined in Sec. V. The angle variable X, defined by (2.4) was set equal to x, the spatial coordinate, for all curves so that we are looking at the wave in a frame of reference moving with the phase speed, c_1. The double cnoidal wave is simply periodic in time in this reference frame with a period $P = 1/c_2$. Solid curve ($t = 0$), dashed curve ($t = P/4$), and dotted curve ($t = P/2$) show one half of a time period. $T_{11} = 0.397$, $T_{12} = 0.359$, and $T_{22} = 0.892$ (with $k_1 = 1$ and $k_2 = 2$, here and in the next three figures).

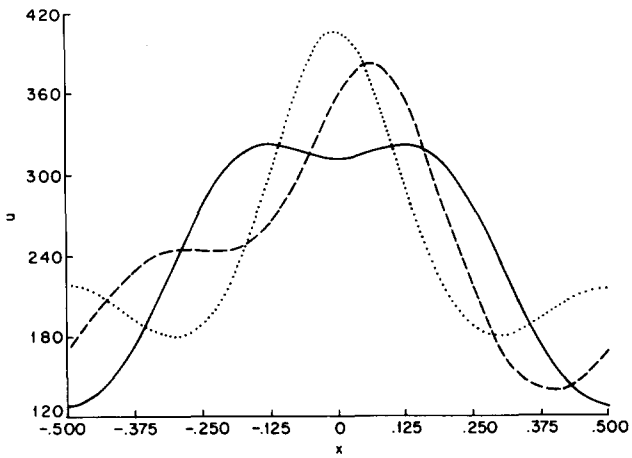

FIG. 3. Same as Fig. 2 except that the polycnoidal wave is in that intermediate parameter range where it can be regarded (and accurately approximated) as either a pair of linear sine waves or a pair of solitary waves. Solid curve ($t = 0$), dashed curve ($t = P/4$), and dotted curve ($t = P/2$), where P is the time period.

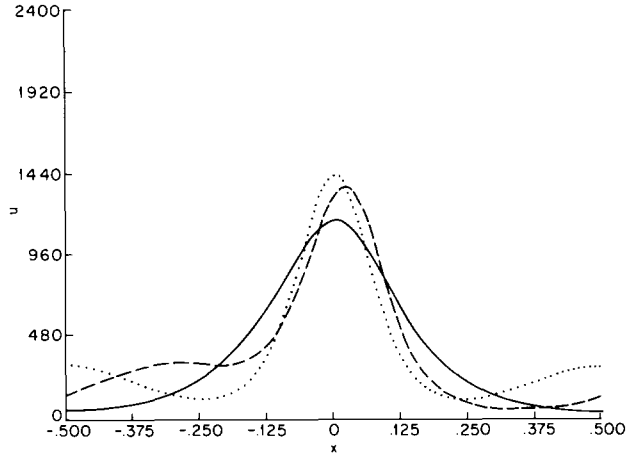

FIG. 4. Same as Figs. 2 and 3 except that the polycnoidal wave is actually a weakly perturbed ordinary cnoidal wave. Solid curve ($t = 0$), dashed curve ($t = P/4$), and dotted curve ($t = P/2$), where $T = 1/c_2$ is the time period. $T_{11} = 1.00$, $T_{12} = 0.759$, and $T_{22} = 3.00$.

lision is a once-in-a-lifetime event, and therefore does not affect the average speed of the solitons. On the periodic domain, the collision is repeated endlessly, so the repeated phase shifting does alter the average phase speed of the solitons. The implications of this are discussed in the next section and more particularly in Sec. V.

Figure 3 shows the double cnoidal wave when both peaks are much smaller and wider. The parameter values are such that the polycnoidal wave lies in that intermediate regime where it can be equally well considered to be a solitary wave or a pair of sine waves: both lowest-order approximations agree with the exact solution to within a few percent of accuracy. The qualitative behavior is very similar to that of the extreme double soliton case shown in Fig. 2, and can likewise be interpreted as colliding solitary waves. The alternative sine wave interpretation is equally straightforward.[17] At $t = 0$ (solid curve, Fig. 3), a trough of the second harmonic is 180 degrees out of phase with the wavenumber one component at $X = 0$. The result is a dimple at $X = 0$, where the peak of the fundamental is partially cancelled by a trough of the second harmonic, two peaks on either side of the origin near nodes of the second harmonic, and very deep troughs at $X = \pm\frac{1}{2}$, where both the fundamental and harmonic have negative maxima. When the second harmonic has moved a quarter unit in X (dotted curve), there is a single tall, narrow peak at $X = 0$ where the fundamental and second harmonic are in phase, and smaller secondary peaks at $X = \pm\frac{1}{2}$ where the narrow crests of the second harmonic rise from the flatter troughs of the fundamental.

Figure 4 illustrates the rather boring case of a single soliton modified by a small superharmonic (wavenumber two) perturbation ($T_{22} \gg T_{11}$, where $k_2 = 2k_1$). Lax has shown[18] that when the two solitons are sufficiently unequal in size, the tall soliton becomes shorter and broader during the collision (i.e., while out of phase with the crest of the perturbation) but the dimple at or near $X = 0$ (so that Figs. 2 and 3 always have two local maxima) does not occur so that there is only a single local maximum for part of each period in time.

Figure 5 shows the other perturbed soliton regime ($T_{11} \gg T_{22}$). This is a cnoidal wave of half-unit spatial period weakly affected by a subharmonic perturbation of unit period. For clarity, a slightly different convention was used than with the preceding three figures: Instead of keeping the phase of X fixed while advancing that of Y by a half unit, the phase of X was decreased by 0.25 while that of Y was increased by 0.25 to trace out half a time period so that the peaks are quasistationary in the graphical frame of reference.

The twin crests of the cnoidal wave do not merge under the influence of the perturbation, but instead execute a small oscillation about their mean positions. This is perfectly consistent with interpreting this case as the collision of two solitons that differ slightly in amplitude. Lax[18] has shown that, in the words of Fornberg and Whitham,[19] "there are always two maxima; the wave approach each other and exchange roles, but then shear away and do not pass through each other." Another way to look at this to examine the dimple at $x = 0$ at the time of the maximum soliton overlap in Fig. 2. As the ratio of the amplitude of the two solitons becomes closer and closer to 1.0, this local minimum at $x = 0$ be-

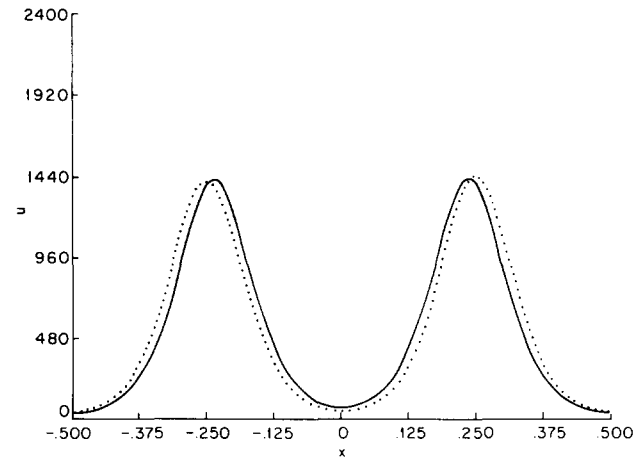

FIG. 5. Same as Figs. 2–4 except that the polycnoidal wave is a simple cnoidal wave of half-unit period subject to a weak perturbation of unit spatial period. For clarity, a different frame of reference was used such that the phase of the angle variable X was decreased by 0.125 between graphs while that of Y was increased by the same amount. Solid curve ($\phi_1 = 0$, $\phi_2 = 0$), dashed curve ($\phi_1 = -0.125$, $\phi_2 = 0.125$), and dotted curve ($\phi_1 = -0.25$, $\phi_2 = 0.25$). $T_{11} = 3.00$, $T_{12} = 0.851$, and $T_{22} = 1.811$.

comes deeper and deeper until the two solitons are separated by a wide, deep trough even at the time of closest approach.

One can also interpret Fig. 5 in terms of constructive and destructive interference between two periodic waves of different phase speeds. Although not obvious on the graph, the right peak in Fig. 5(b) is in fact slightly taller than the left peak as a result of constructive interference at $x = 0.25$ with the crest of the $k_1 = 1$ component while the left soliton is shrunk a bit because it rests on the trough of the perturbation at $x = -0.25$. As the perturbation continues to move relative to the tall peaks, it will reinforce and weaken each large crest in turn. Thus, one has two alternative interpretations of this case that lead to the same conclusions: (i) two colliding solitary waves of almost identical amplitude on each periodicity interval, or (ii) a simple cnoidal wave of half-unit period whose crests swell and accelerate or shorten and slow down as the crests and troughs of the sine wave perturbation move through them.

IV. THE GEOMETRY OF THE X-Y PLANE

Although the samples of the preceding section illustrate the general characteristics of double cnoidal waves, there are some important, but subtle, aspects of polycnoidal waves which can be explained only by examining $\theta(X,Y)$ and its relation to $u(x,t)$. As noted in Ref. 1, a heuristic way of constructing a polycnoidal wave is to simply repeat the usual multiple soliton solution over the whole x-axis. The resulting approximation is obviously periodic, but generally is not an exact[20] solution of the Korteweg–de Vries equation.

Boyd[1] shows, however, that Hirota's transformed single solitary wave solution,

$$F = 1 + \exp(2sX), \tag{4.1}$$

which gives the usual hyperbolic secant squared soliton upon taking the second logarithmic derivative, can be generalized to a "bi-Gaussian"

$$\Theta(x,t) = \exp[-s(X - \pi/2)^2/\pi] + \exp[-s(X + \pi/2)^2/\pi]. \tag{4.2}$$

If one repeats (4.2) over the whole interval, one obtains the Gaussian series of the one-dimensional theta function, which is an exact solution of the Hirota–Korteweg–de Vries equation, and therefore generates an exact solution of the KdV equation upon taking the second logarithmic derivative. Figure 6, which is borrowed from Boyd,[6] illustrates the procedure. The shape of the polycnoidal wave is determined by the theta function; the only remaining unknown (for the ordinary cnoidal wave) is to solve a pair of algebraic equations to determine the nonlinear phase speed c_1 in the "angle" variable X.

The same concept applies for higher polycnoidal waves. In particular, a "tetra-Gaussian" consisting of four Gaussian functions of identical shape but with peaks located at the four corners of a unit square ($X = \pm 0.5$, $Y = \pm 0.5$) gives the usual double soliton of the KdV equation on an infinite domain in x. (A proof is given in Appendix B of Ref. 6.) When this tetra-Gaussian is repeated with unit spacing over the whole of the X-Y plane, it generates the Gaussian series of the theta function.

In the near-double soliton regime (small T_{11}, T_{22} or

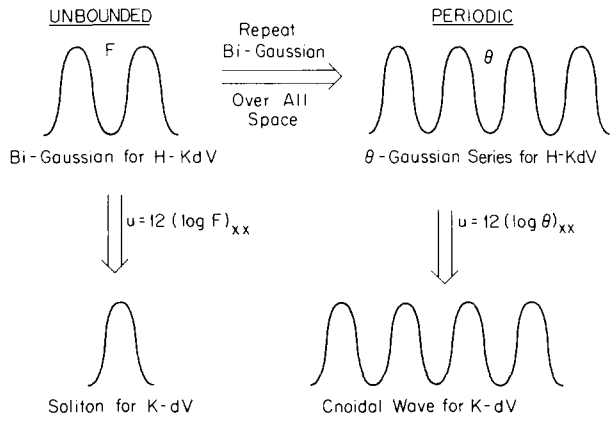

FIG. 6. Schematic diagram showing the relationship between the bi-Gaussian and theta function solutions to Hirota's transformed version of the KdV equation. The left side shows the situation when the domain is unbounded: The solution to the transformed KdV equation has just two peaks on all of $X \in [-\infty, \infty]$, and the second logarithmic derivative of this gives a single crest (corresponding to the valley betwen the two peaks of the bi-Gaussian) which is the usual solitary wave. When the bi-Gaussian pattern is repeated with even spacing over all X, it generates the Gaussian series of the theta function. This, as shown on the right, is a spatially periodic solution of the transformed KdV equation and its second logarithmic derivative is the simple ($N = 1$) cnoidal wave. [Taken from Boyd[1].] For the double cnoidal wave, the basic unit is a tetra-Gaussian with peaks at the four corners of a unit square in the X-Y plane which generates the double solitary wave when the domain is unbounded. The idea is the same, however, repeating this basic unit over all of X-Y space with even spacing gives a periodic solution to the transformed KdV equation whose second logarithmic derivative with respect to x is the double KdV cnoidal wave.

equivalently, large R_{11} and R_{22}), the Gaussians are sharply peaked so that the full infinite series can be approximated on the unit square by the sum of the four Gaussians whose peaks are at its corners. The reason that it is not possible to approximate the series by a single Gaussian is that $u(x,t)$ is obtained by taking the second logarithmic derivative, which for a single Gaussian would be $u(x,t) = \text{const}$. The solitons actually lie in the valleys between the peaks of the Gaussians, and the center of the square where the two valleys meet is also where the solitons collide.

Figure 7 shows the graph of the theta function in the X-Y plane with the contours of the function

$$U(X,Y) = 12\{k_1^2(\log\theta)_{XX} + 2k_1k_2(\log\theta)_{XY} + k_2^2(\log\theta)_{YY} + \alpha\} \tag{4.3}$$

also plotted. (The constant α has been added so that the solitons asymptote to 0, as in Figs. 2–5.) The function $u(x,t)$ which actually solves the KdV equation is obtained from $U(X,Y)$ by drawing a line of slope k_2/k_1 through the origin ($X = 0$, $Y = 0$). The values of $U(X,Y)$ along this line then give the values of $u(x,t=0)$. The function $u(x,t)$ is obtained at later times by moving the line with the velocity $-c_1$ in X and $-c_2$ in Y consistent with the definitions (for $k_1 = k_2 = 1$)

$$X = x - c_1t, \quad Y = x - c_2t. \tag{4.4}$$

[The reason for the minus signs is so that $u(x = 0,t) = U(-c_1t, -c_2t)$ and similarly for other x to agree with (4.4).]

If the solitary waves collided without a shift of phase, then (i) the theta matrix and inverse theta matrix would be diagonal, i.e., $T_{12} = R_{12} = 0$; (ii) the ridges of $U(X,Y)$ would be parallel to the X and Y axes. In reality, however, there is a

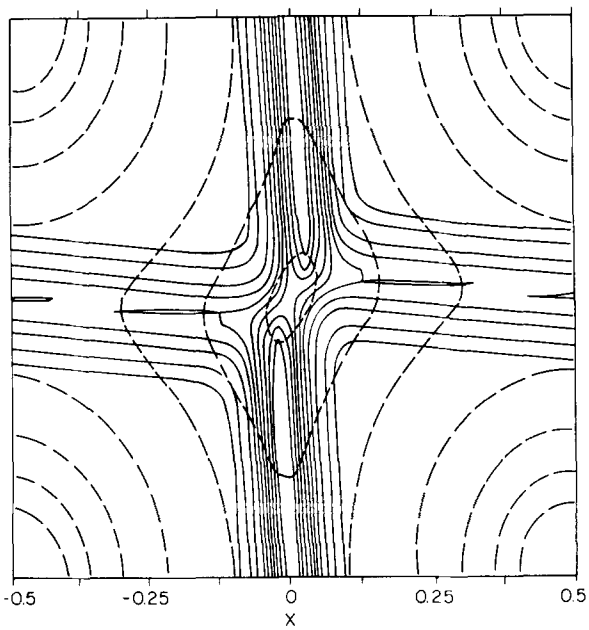

FIG. 7. Contours of the two-dimensional theta function (dashed lines) and of $U(X,Y)$ in the unit square whose corners are $X = \pm 0.5$ and $Y = \pm 0.5$. This is in the double solitary wave regime; the Gaussian series was used with $k_1 = k_2 = 1$, and $R_{11} = 50$, $R_{12} = 2.913$, and $R_{22} = 30$. The function $u(x,t)$ for this case is shown in Fig. 2.

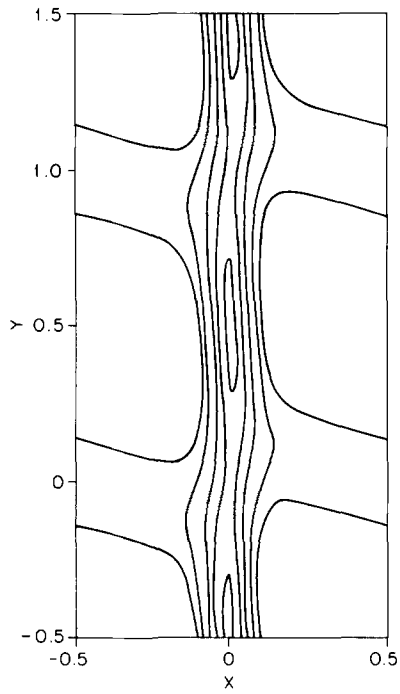

FIG. 8. Contours of $U(X,Y)$ in the rectangle whose corners are $X = \pm 0.5$ and $Y = 0.5, +1.5$ for $k_1 = 1$ but $k_2 = 2$. When converted from X and Y to the actual spatial coordinate X, all of this rectangle projects onto a unit interval in x. $R_{11} = 32$, $R_{12} = 2.20$, and $R_{22} = 8$. The corresponding $u(x,t)$ is shown in Fig. 9.

phase shift of both solitary waves after the collision—the taller soliton is temporarily accelerated while the shorter one is deaccelerated during their encounter—so the ridges of $U(X,Y)$ are tilted with respect to the axes. The magnitude of the slope is given in Appendix C of Ref. 6 along with other formulas describing the contours of $U(X,Y)$ and so on, but the mere fact of the slope is enough to show one rather startling fact: The phase velocities c_1 and c_2 are not the speeds at which the solitons travel when outside the collision region.

In the next section, the reason will be discussed in detail. In brief, one concludes that c_1 and c_2 represent the average velocities of the two solitary waves, and these averages are changed from the usual noncolliding soliton speeds because of the phase shifts that occur during the collision. When the spatial domain is unbounded and there are but two solitons, the collision occurs but once. With spatial periodicity, the collisions recur endlessly and the average speed of the solitons is altered. Before turning to this, however, we must first explore the role of wavenumbers.

Figure 7, which shows a unit square in the X-Y plane, implicitly assumes $k_1 = k_2 = 1$. When $k_2 = 2$, however, Y varies by 2 when x varies by 1. Thus, for $k_1 = 1$ but $k_2 = 2$, the whole of the rectangle shown in Figure 8 projects on a unit interval in x. The line which takes $U(X,Y)$ to $u(x,t)$ now has a slope of 2, and the reader can see (by laying a ruler between the lower left and upper right corner) that for part of each temporal period, there are three solitons on each unit interval in x: one tall solitary wave and two short solitary waves. Figure 9 shows $u(x,t)$ for the same wave as in Fig. 8. Thus, the wavenumbers are extremely important in determining the qualitative nature of the flow, and Sec. VI will examine that role in detail.

V. PHASE SPEEDS AND SOLITON VELOCITIES

As shown in Ref. 6, the overlap of the solitons on one unit periodicity interval in x with those of another creates corrections to c_1 and c_2 which can be calculated as a double perturbation series in the parameters $\exp(-R_{11})$ and $\exp(-R_{22})$. Since the solitons decay exponentially with x [as $\exp(-R_{11}|x|)$ and $\exp(-R_{22}|x|)$], it follows that these "overlap" corrections decrease exponentially with the half-widths of the solitary waves. The differences between c_1 and c_2 and the velocities of the solitons, however, decrease only linearly with the widths of the solitons, and are therefore

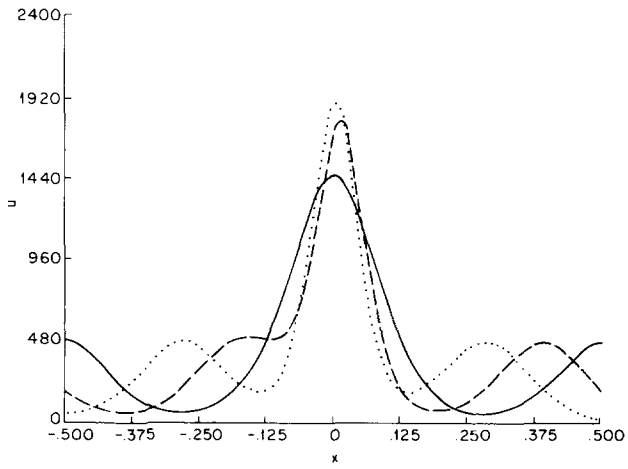

FIG. 9. The KdV solution $u(x,t)$ for the wave whose theta function is plotted in Fig. 8. As with Figs. 2–4, the phase of X is kept fixed so that we view $u(x,t)$ in a frame of reference moving with the phase velocity c_1. In this reference frame, the wave is periodic in time with a period $P = 1/c_2$. Solid curve ($t = 0$), dashed curve ($t = P/4$), and dotted curve ($t = P/2$).

something quite different in nature.

One proof of this comes from the observation that the slopes of the ridges of $U(X,Y)$, which are responsible for making the phase and soliton velocities differ, are given by $-R_{11}/R_{12}$ and $-R_{12}/R_{22}$, respectively, as shown in Appendix C of Ref. 6. Since R_{12} remains $O(1)$ when R_{11} and R_{22} become large, it follows that the slopes of the soliton ridges in the X-Y plane become increasingly parallel to the Y and X axis, respectively. The angles between the solitons and the axes, however, are linear functions of $1/R_{11}$ and $1/R_{22}$ while the "overlap" corrections, i.e., the higher-order terms in the perturbation series of Ref. 6, are decreasing exponentially in these same variables.

A more direct way is to simply calculate these quantities to zeroth order in perturbation theory, which is equivalent to truncating the infinite theta function series to the minimum of four Gaussian functions needed to generate the double solitary wave. It is shown in Ref. 6 that the phase velocities c_1 and c_2 that appear in the "angle" variables X and Y are obtained from the "pseudofrequencies" ϵ_1 and ϵ_2 by solving the pair of linear equations

$$\begin{vmatrix} (-R_{11}k_1) & (-R_{12}k_2) \\ (-R_{12}k_1) & (-R_{22}k_2) \end{vmatrix} \begin{vmatrix} c_1 \\ c_2 \end{vmatrix} = \begin{vmatrix} \epsilon_1 \\ \epsilon_2 \end{vmatrix}. \tag{5.1}$$

To lowest order

$$\epsilon_i = -c_i^{\mathrm{sol}}\delta_i, \quad i=1,2, \tag{5.2}$$

where

$$\delta_i \equiv R_{ii}k_i + R_{12}k_j, \quad i=1,2,\ j\neq i \tag{5.3}$$

gives the width of each soliton and where c_i^{sol} is the "free" velocity of a soliton, i.e., the speed at which the soliton travels when not in collision with another. When "free," $u(x,t)\simeq 3\delta_i^2\,\mathrm{sech}^2[\delta_i(x-c_i^{\mathrm{sol}}t)]$ in the neighborhood of the ith soliton. If we add a constant[16] to $u(x,t)$ and the phase speeds so that the solitons asymptote to 0 for large x—the result is still a polycnoidal wave solution of the KdV equation—then

$$c_i^{\mathrm{sol}} = \delta_i^2, \quad i=1,2 \tag{5.4}$$

which is the usual formula as given in Whitham,[21] for example, although he uses κ in place of our δ.

Through elementary algebra, one can show from (5.1) through (5.4) that

$$c_1 = c_1^{\mathrm{sol}} + \frac{(c_1^{\mathrm{sol}} - c_2^{\mathrm{sol}})R_{12}\delta_2}{k_1(R_{11}R_{22} - R_{12}R_{12})}. \tag{5.5}$$

In the extreme soliton regime (R_{11}, $R_{22}\gg 1$), R_{11}, $R_{22}\gg R_{12}$, which permits (5.5) to be simplified to

$$c_1 = c_1^{\mathrm{sol}} + (c_1^{\mathrm{sol}} - c_2^{\mathrm{sol}})k_2\{R_{12}/\delta_1\}. \tag{5.6}$$

Now it can be shown (Whitham[21] and Appendix C of Ref. 6) that the phase shift experienced by a soliton of amplitude determined by R_{11} (which we shall call "type 1" for short) after collision with a soliton of the other size is (R_{12}/δ_1), so (5.7) implies, reasonably enough, that the difference between the "free" speed of the soliton and the corresponding phase velocity in X is proportional to this phase shift—which argues strongly that it is the phase shift that is the cause of this difference. If this explanation is correct, however, then (5.6) should also depend upon the frequency with which a soliton of type 1 collides with a soliton of type 2. Since k_2 determines the number of solitons of type 2 per unit interval in x, it follows that $k_2(c_1^{\mathrm{sol}} - c_2^{\mathrm{sol}})$ is the frequency with which a soliton of type 1 will collide with a soliton of the other size per unit time. The wavenumber k_1, which determines the density of type 1 solitons per unit interval of x, is conspicuously missing from (5.6); it has no bearing on the number of collisions between a particular soliton of type 1 and all the solitons of the other height because a type 1 soliton collides only with the solitary waves of the other amplitude. Thus, (5.6) can be rewritten schematically as

$$c_1 = c_1^{\mathrm{sol}} + \{\text{number of collisions/unit time}\}\{\text{phase shift/collision}\} \tag{5.7}$$

and similarly for c_2.

Thus, as mentioned earlier, c_1 and c_2 may be properly interpreted as the average speeds of the solitary waves while their instantaneous speeds (outside collision zones) are given by the different quantities c_1^{sol} and c_2^{sol}.

VI. WAVENUMBERS AND THE SPECIAL MODULAR TRANSFORMATION

The wavenumbers k_1 and k_2 have different roles in the double-sine wave and double-soliton regime. In the near-linear regime, k_1 and k_2 are the actual wavenumbers of the two sinusoidal, noninteracting waves that approximate the polycnoidal wave. In the double-soliton regime, the widths of the solitary waves are given by the "pseudowavenumbers" defined by (5.3) above, and k_1 and k_2 instead give the number of solitons on each interval. This was shown explicitly by Figs. 8 and 9 in Sec. IV, where a double cnoidal wave with three solitons on each unit interval was displayed. Since $R_{11} > R_{22}$ for this case and k_2 was the wavenumber equal to two, the pair of identical solitons was shorter than the third, but one could mix two tall solitons with a single shorter one on each unit interval by either choosing $k_1 = 2$ instead or taking R_{22} larger than R_{11}. More exotic combinations are possible and it will be argued in the next section that Hyman[22] computed a double cnoidal wave with four solitary waves on each spatial period, three tall and one short.

This all seems rather straightforward, but in reality the issue of wavenumbers is so complicated as to demand an entire separate article unto itself (Ref. 7). The Serpent in Eden is that the different roles assigned to the wavenumbers for solitons and sine waves are contradictory. Figures 7–9 show clearly that the usual situation of two solitons of unequal size per unit interval in x demands $k_1 = k_2 = 1$, but in the sine wave regime, this is absurd because the linear dispersion relation demands that two infinitesimal amplitude waves of the same wavenumber must also have the same phase speed, and the double cnoidal wave collapses into the ordinary single cnoidal wave. The simplest possibility that preserves two distinct phase speeds and "phase" variables and is a true double cnoidal wave is to take $k_2 = 2k_1$, i.e., one wave is the second harmonic of the other.

The resolution of this difficulty lies in a remarkable fact that at first seems only to put us into more trouble: Each theta function of two or more dimensions can be written in a

denumerable infinity of ways via the so-called "special modular transformation" which is the central theme of Ref. 7. The theta matrices and wavenumbers are transformed by matrices whose elements are integers so that the equivalent representations of a theta function with integral wavenumbers are restricted to those for which the new wavenumbers are integers also.

Physically, of course, there is no ambiguity at least in the limits of very large or very small wave amplitudes: In the double-soliton regime, there is only one representation for which the wavenumbers give the actual density of solitary waves on the unit interval and the phase speeds of the phase variables are the average velocities of the solitons, and in the double-sine wave regime, there is again only one way of writing the theta function in which the wavenumbers and phase speed of its arguments X and Y are the actual wavenumbers and phase speeds of the two sine waves. The special modular transformation is thus a way of providing the theta function with a mathematical disguise which alters the arguments and parameters of the theta function without altering the Korteweg–de Vries solution which it generates. It would be quite foolish, however, to dismiss the modular transformation as a mere mathematical curiosity.

In the first place, it implies that the nonlinear implicit dispersion relation given in Ref. 6, which must be solved to determine c_1, c_2, and the diagonal theta matrix element, has nonunique solutions. (In fact, an infinite number of them.) Some care is needed to insure that one computes in the "physical" representation so that the phase speeds computed are those of the actual components of the polycnoidal wave being sought, and not merely mathematical disguises for something quite different.

In the second place, the special modular transformation resolves the dilemma of needing different wavenumbers to make sense of the simplest double-soliton and double-sine wave regimes. If one solves the residual equations by varying the diagonal theta matrix elements in small steps, the so-called "continuation" method, one finds upon graphing $u(x,t)$ that the mode which is the sum of one sine wave with $k_1 = 1$ plus another with $k_2 = 2$ does indeed smoothly continue into a pair of solitary waves, one tall and one short, on each unit interval. The phase speeds so computed, however, are not those of the actual solitons, but can be made into them by taking that modular transformation which reduces the wavenumber from $k_2 = 2$ to $k_1 = 1$. In a similar way, if one begins with the double soliton for $k_1 = k_2 = 1$ and marches in the opposite direction of decreasing amplitude, the phase speeds computed from the residual equation will not be those of the sine wave and its second harmonic that dominate $u(x,t)$ when the amplitude is small, but can be changed into the physical wave speeds through the modular transformation that sends k_2 from 1 to 2. The whole business is discussed thoroughly with numerical tables in Ref. 7.

The modular transformation makes it necessary to introduce some notation. A pair of numbers written in square brackets, for example, [1,2], is used to denote the wavenumbers of the Fourier representation with k_1 written first. A superscript "P" can be added to denote that the "physical" representation is meant and not one of the infinite number of disguises allowed by the mathematics. (When there is no danger of confusion, the superscript P will be omitted; when this notation is used elsewhere in this series of papers, the "physical" representation will always be meant unless expressly stated otherwise.) In a similar way, curly brackets, i.e., $\{1,1\}$ will be used to denote the wavenumbers of the Gaussian series of the theta function. The author apologizes for burdening physics with more notation, but it is unavoidable. It is necessary to introduce separate notation for the Fourier and Gaussian series because

$$[1,2]^P = \{1,1\}^P. \tag{6.1}$$

In words, the mode which is the sum of a wave and its second harmonic for small amplitude is the sum of one tall and one short solitary wave for large amplitude.

Reference 7 goes on to describe in some detail the identifying characteristics of the "physical" representation. First, it is that for which the off-diagonal theta matrix element is small in comparison to the diagonal theta matrix elements. Second, it is the representation employed by the perturbation series of Ref. 6—the perturbation series always give answers in the "right" representation, in other words. The perturbation series suggest T_{12} and R_{12} are always positive, so a representation in which either of these off-diagonal elements is negative is almost certainly not the physical representation.

Finally, one can give a graphical definition. Figure 10 compares $U(X,Y)$ for two different $\{1,2\}$ modes. The left panel is simply a repeat of Fig. 8; the corresponding $u(x,t)$ is given by Fig. 9 and truly has three solitary waves on each unit interval in x. The right panel, however, is in an unphysical representation. Notice that the repeated soliton ridges have a steep positive slope rather than a shallow negative slope as in the left panel. The reason is that R_{12} is large and negative instead of being small and positive as it should be.

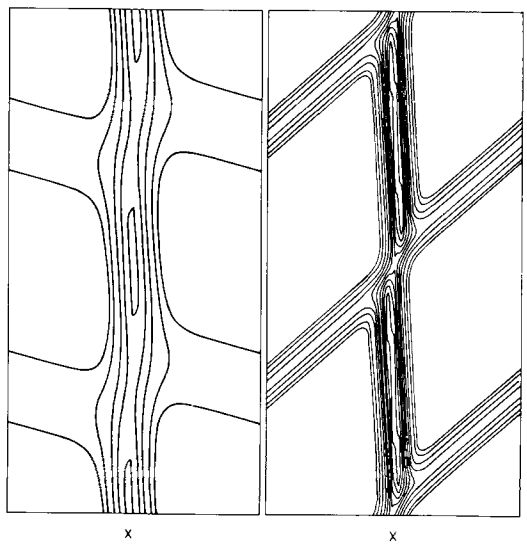

FIG. 10. Contours of $U(X,Y)$ for two theta functions with $k_1 = 1$ and $k_2 = 2$. (a) [left panel] This is identical with that shown in Fig. 8; this choice of wave numbers is the physical representation of this wave, so this mode is denoted $\{1,2\}^P$. (b) [right panel] This is actually a $\{1,1\}^P$ mode in disguise with $R_{11} = 74.17$, $R_{12} = -27.09$, and $R_{22} = 30$. Although (b) looks quite different from Fig. 7, they are plots of the same theta function in different representations; when the function shown in (b) is converted back into (x,t) coordinates, the resulting $u(x,t)$ is that shown in Fig. 2.

By laying a ruler across the figure at a slope of k_2/k_1, i.e., 60 degrees, one can convince oneself that even though one wavenumber is 2, there are in fact no more than two solitons present at any time. The actual $u(x,t)$ for Fig. 10(b) is in fact that graphed in Fig. 2.

VII. PREVIOUS CALCULATIONS OF DOUBLE CNOIDAL WAVES

Although there have been a huge number of abstract, theoretical papers on polycnoidal waves, there have been only two explicit attempts to calculate and graph KdV polycnoidal waves before this present work. Both have limitations which illustrate the usefulness of the ideas developed in the two companion papers (Refs. 6 and 7).

Hyman[22] used a variational principle of Lax' to numerically calculate a number of case studies of double cnoidal waves, although only one is described in detail in his paper. By carefully computing the trajectory of the maxima, he showed "the peaks move with two distinct speeds. In any spatial period three of the peaks are traveling with one speed while the fourth is traveling faster." This inspired the remark by other researchers,[23] "The general shape [of $u(x,t)$] is still obscure, though a large body of numerical information has been obtained by J. M. Hyman; for example, he finds that for $N = 2$, the number of peaks and valleys is usually 4 and on occasion 5." The case illustrated in Hyman's own paper has 4 peaks and 4 valleys.

In light of what has been presented earlier here, it is difficult to escape the conclusion that Hyman actually computed only double cnoidal waves with the physical representation $\{1,3\}^P$, i.e., four solitons on each unit interval with three of one size and a fourth of another, and missed the $\{1,2\}^P$ or $\{1,1\}^P$ modes. Figures 2 through 5 show clearly that the conclusion that the "number of peaks and valleys is usually four" is nonsense; the $\{1,1\}^P - [1,2]^P$ mode has only two peaks and two valleys, sometimes less. The conclusion would seem to be that Lax' variational principle combined with numerical nonlinear optimization is a poor way to investigate polycnoidal waves.

Hyman's paper is still of interest, however, because he superimposed random perturbations upon his double cnoidal waves and found them to be remarkably stable. It seems probable that this is true of all polycnoidal waves, but a proof is lacking, and Hyman's paper is at present the only evidence in favor of this hypothesis.

Hirota and Ito[8] have computed a double cnoidal wave by numerically solving the implicit dispersion relation. Table I gives their results in their original notation, translates their results into the notation used here, and then compares the results with the Fourier and Gaussian perturbation series derived in Ref. 6. The result is a rather resounding triumph for perturbation theory: The second-order Fourier series gives all three physically significant unknowns to within 4% relative error while the zeroth order Gaussian series, i.e., the tetra-Gaussian double soliton, gives these same three quantities to within 4% error also. The conclusion is that number crunching is not really necessary: for most purposes, the perturbation series of Ref. 6 are more than adequate.

TABLE I. A comparison of the numerical calculations of a double cnoidal wave from Hirota and Ito[8] with Fourier and Gaussian perturbation theory. The first line of the table gives the numerical results of Hirota and Ito in their own notation. The second line gives the same exact solution in terms of the notation and conventions employed here. (Their theta matrix elements must be multiplied by π, their constant of integration λ divided by -2 to give my A, and their frequencies converted into phase speeds by multiplying by $-1/k_1$. Because I normalize k_1 to 1, it is also necessary to multiply the phase speeds by 6.25^2 and A by 6.25^4 to increase the wavenumbers by a factor of $6.25 = 1/0.16$.) The third part of the table gives the results of Fourier perturbation theory; because of the smallness of the nome $q_2 \sim q_1^2$, the terms in q_2^2 were neglected in computing the first-order solution and q_2^4 in the second-order solution. Relative errors are given in square brackets. The fourth part of the table gives the results of Gaussian perturbation theory for $R_{11} = 14.38$, $R_{22} = 6.478$, which correspond to the T_{11} and T_{22} values employed in the rest of the table. Normally, it would be necessary to determine these R_{11} from the corresponding T_{11} through some kind of iterative procedure as explained in the text.

Hirota–Ito Notation

k_1	k_2	τ_{11}	τ_{22}	λ	ω_1	ω_2	τ_{12}
0.16	0.32	0.464	1.16	−2.01	−0.086	1.23	0.297

Boyd Notation

k_1	k_2	T_{11}	T_{22}	A	c_1	c_2	T_{12}
1.0	2.0	1.458	3.64	1 533	21.00	−150.2	0.933

Fourier Perturbation Theory

	A	c_1	c_2	T_{12}
0th order	0 [100%]	−39.5 [300%]	−157.9 [5.2%]	1.099 [17.8%]
1st order	1 013 [34.5%]	11.8 [43.5]	−157.9 [5.2%]	0.936 [0.27%]
2nd order	1 547 [0.89%]	20.2 [3.8%]	−150.4 [0.15%]	0.933 [<0.1%]

Gaussian Perturbation Theory

	A	c_1	c_2	R_{12}
0th order	1 443 [5.8%]	20.3 [3.6%]	−149.0 [0.79%]	2.335 [0.56%]

Their paper, however, is of further interest because it also computes a triple cnoidal wave. This has only seven unknowns but there are *eight* residual equations. Knowing from the "Hill's spectrum method" that theta function solutions should exist, they boldly chose seven of the eight equations and solved them as a closed system, and then verified after the fact that the extra equation was also satisfied to within machine precision. It would be extremely interesting to have an analytical proof of the redundancy of the residual equations for $N = 3$ and higher, as opposed to their numerical proof, but none is yet known.

Thus, although the analysis of Refs. 6 and 7 makes it possible to improve on these early, limited calculations by Hyman and by Hirota and Ito, both papers are still valuable for their intelligent use of numerical solutions to suggest as yet unproven theorems for the future.

VIII. THE DOUBLE CNOIDAL WAVE IN PERSPECTIVE

The methods employed here and in Refs. 1, 6, and 7 can be extended, with a few additional tricks, to most or all of the "exactly integrable," soliton-admitting equations which are now known to be solvable via theta functions through the "Hill's spectrum" method. The Korteweg–de Vries equation is one of several whose Hirota-transformed equivalent is a single bilinear differential equation: applying the new algorithms to the Boussinesq equation,

$$u_{tt} - u_{xx} - u_{xxxx} - [u^2]_{xx} = 0, \tag{8.1}$$

for example, is merely a matter of altering the function $\zeta(p,q)$ which is defined in Ref. 6. Other soliton equations like the sine-Gordon equation and cubic Schrödinger equation have Hirota equivalents which are systems of bilinear equations rather than a single equation. For these, there are still some holes even in the Hill's spectrum method, so the class of "coupled bilinear" equations requires further work. Still, there seems little doubt that most of the concepts developed here (using the Gaussian series for large amplitude and the Fourier series for small, reducing the partial differential equation to the algebraic residual equations, computing explicit perturbation series, and applying the modular transformation) will be important for these other types of soliton equations, too.

A much harder question is to relate the KdV polycnoidal waves to the nonlinear solutions of similar differential equations that are not "exactly integrable" via the inverse scattering or Hill's spectrum algorithms. The Gaussian series, which converges most rapidly when the wave amplitude is large, is a specific property of theta functions and does not carry over to waves that cannot be described in terms of theta functions.

Reference 1 (Appendix B) has shown, however, that it is possible to compute Fourier series representations for polycnoidal waves by using Stokes' expansions, which is a particular case of the singular perturbation technique known as the "method of multiple scales," without employing theta functions in any sense at all. The Stokes' expansion strongly suggests that double and triple and N-polycnoidal waves exist for almost any species of neutral, nondissipative waves whether the governing equation is "exactly integrable" or not.

This hypothesis must be qualified in several obvious ways. First, a perturbation series for a wave is not quite the same thing as an existence proof for the wave. For the Korteweg–de Vries equation, the Hill's spectrum method shows that the theta series converges for all values of the wave amplitude; the corresponding Fourier series for a nonintegrable equation may have only a finite radius of convergence, or perhaps be an asymptotic series with no radius of convergence at all.

Second, numerical experiments with nonintegrable differential equations have shown that their solitons collide inelastically with often the creation of a new soliton or the permanent destruction of an old one; such solutions cannot be classified as (limiting cases of) polycnoidal waves. However, this does not contradict the hypothesis that polycnoidal waves exist for nonintegrable equations, too. What makes polycnoidal waves so important for the Korteweg–de Vries equation is that they are complete, that is, the general initial value solution can be approximated to an arbitrary degree of accuracy by an N-polycnoidal wave of sufficiently large N. It seems probable that polycnoidal waves exist for at least some nonintegrable partial differential equations, but lack this property of initial value completeness. In other words, for nonintegrable equations, there are solutions which cannot be approximated to arbitrary accuracy by polycnoidal waves.

It is known, however, that for some nonintegrable equations which are closely related to integrable equations, the degree of inelasticity seems to be small. (This notion of "nearly integrable" equations is well developed with many examples in the review by Makhankov.[24]) Perhaps with better understanding of polycnoidal waves, it will be possible to put a bound on the nonpolycnoidal part of the solution and still apply the concept of a polycnoidal wave, at least qualitatively, to such nearly integrable equations.

IX. SUMMARY AND CONCLUSIONS

This article and its two companions (Boyd[6,7]) have tried to show that much can be learned about the generalized cnoidal waves of the Korteweg–de Vries equations and related equations by using rather elementary methods. The perturbation series of Boyd[6] provide an accurate means of calculating both phase speeds and $u(x,t)$ itself in all the interesting parameter regimes. The Gaussian series is especially useful because it converges rapidly in precisely that domain—large amplitude—where all normal perturbation theories fail. The special modular transformation, which involves nothing more esoteric than multiplying the theta matrix by another matrix whose elements are explicitly given integers, is essential in correctly interpreting the various modes of the double cnoidal wave. The most important mode is shown to be the sum of two solitary waves on each unit interval in x for large amplitude and to be the superposition of two linear sine waves, with one being the second harmonic of the other, for small amplitude.

The directions of future research are fairly clear. One is to simply apply the formalism developed here to other soliton equations like the Boussinesq equation (8.1) and turn the crank.

A second, more interesting direction is to explore the

connection between polycnoidal waves and the general initial value problem with spatial periodicity. The Hill's spectrum method provides one complicated and indirect means of calculating that polycnoidal wave which approximates a given, arbitrary initial condition. It is known, however, that one can obtain a simpler answer by employing the method of multiple scales (a Stokes' expansion-with-a-twist, if you will) for small amplitude, and it appears possible to extend this into an effective numerical algorithm for any amplitude.

A third line of attack is to explore those other soliton equations whose Hirota bilinear form is a pair of equations rather than just one. The sine-Gordon equation and the cubic Schrödinger equation are examples. There are still some gaps even in the Hill's spectrum theory for these equations, so the extension of the ideas presented here to the coupled-bilinear class of systems is far from trivial. Nonetheless, one expects that perturbation theory, Gaussian series, the algebraic residual equations, and the modular transformation will all play a role.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation through grants OCE 8108530 and OCE 8305648.

APPENDIX A: THETA FUNCTION NOTATION

Mathematicians normally define the theta function via

$$\theta\begin{bmatrix}\boldsymbol{\epsilon}\\ \boldsymbol{\epsilon}'\end{bmatrix}(\boldsymbol{\zeta},\mathbf{T}) = \sum_{\mathbf{n}} \exp\left\{\pi i\left[\sum_{i=1}^{N}\sum_{j=1}^{N} t_{ij}\left(n_i+\frac{\epsilon_i}{2}\right)\right.\right.$$
$$\left.\left.\times\left(n_j+\frac{\epsilon_j}{2}\right)+2\sum_{i=1}^{N}\left(n_i+\frac{\epsilon_i}{2}\right)\left(\zeta_i+\frac{\epsilon_i'}{2}\right)\right]\right\}. \tag{A1}$$

$\boldsymbol{\zeta}$ is the N-dimensional vector of dependent variables; in the theory of polycnoidal waves, $\zeta_1 = k_i(x-c_it)+\phi_i$, $i=1,\ldots,N$ as in (1.1). The quantity $\begin{bmatrix}\boldsymbol{\epsilon}\\ \boldsymbol{\epsilon}'\end{bmatrix}$, the "characteristic" of the theta function, consists of two N-dimensional row vectors written one above the other with each element restricted to be either 0 or 1. The vector $\mathbf{n}=(n_1,n_2,\ldots,n_N)$, and the summation is taken over all possible positive and negative integers (including 0) for each of $n_1,n_2,\ldots,n_N$.

In applications to KdV polycnoidal waves, one can pick the characteristic at will. The usual choice, as in Nakamura[5] and Boyd,[1] is to use $\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix}(\boldsymbol{\zeta},\mathbf{T})$. For the Gaussian series (soliton regime calculations), the formulas are a little simpler if one employs

$$\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix}(\boldsymbol{\zeta},\mathbf{T}) = \theta\begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix}\left(\boldsymbol{\zeta}+\frac{1}{2},\mathbf{T}\right). \tag{A2}$$

Note that the two differ only in choice of the phase of $\boldsymbol{\zeta}$, but like all wave phases, these are arbitrary anyway. The choice of theta characteristic is physically irrelevant.

Although Ref. 7 uses the theta matrix in the mathematician's form (A1) [for convenience in discussing the derivation of the "special" modular transformation from the general transformation given by Rauch and Farkas[25]], it is easier in most applications to eliminate the factor of πi by defining the real theta matrix elements

$$T_{ij} \equiv -\pi i t_{ij}. \tag{A3}$$

For the ordinary cnoidal wave $T_{11}\equiv\pi/s$, where s is the parameter used in Ref. 1.

For the Gaussian series, it is similarly convenient to define the elements R_{ij} of a square matrix $\mathbf{R}$, where

$$\mathbf{R} = 2\pi^2\mathbf{T}^{-1}, \tag{A4}$$

$$\mathbf{T} = 2\pi^2\mathbf{R}^{-1}, \tag{A5}$$

where $\mathbf{T}$ in (A4) and (A5) is the matrix whose elements are T_{ij}. The factors of π in (A4) arise from the factor of π in (A1) and (A3) and also from a similar factor of π when the Gaussian series of the theta function is expressed in terms of the inverse of the matrix whose elements are t_{ij}. The factor of 2 is inserted into (A4) to eliminate a huge number of 2's that would otherwise appear in the formulas of the Gaussian series perturbation theory.

APPENDIX B: CORRECTIONS AND CLARIFICATIONS FOR BOYD[1]

This earlier paper contains a number of typographical errors. A comma should be inserted between n' and c on the left-hand side of (6.6). The letter $\boldsymbol{\delta}$ in the argument of θ on the left-hand side of (7.1) should be replaced by $\boldsymbol{\zeta}$. In Eq. (5.3), 12 sech^2 [sX] should be $12s^2$ sech[sX]. In (7.9), a Gaussian factor was omitted from the right-hand side of (7.9); the correct transformation is given by (2.10) of Ref. 7.

The author's earlier article makes the remark (p. 384) that "it is conventional to define the multidimensional theta function so that it is periodic with period 2." This is technically true for the general theta function, but it is somewhat misleading since the special cases $\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix}$ and $\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix}$—the only ones needed for polycnoidal theory—are periodic with period 1, as true of all the solutions discussed in this present, later article and its companions (Refs. 6 and 7).

Finally, as noted in Ref. 20, Toda showed the ordinary cnoidal wave has the exact series representation

$$u(x,t) = \frac{-24s}{\pi} + 12s^2\sum_{\substack{n=-\infty\\ [\text{integers}]}}^{\infty}\operatorname{sech}^2[s(X-n\pi)]. \tag{B1}$$

The remark in Ref. 1 that repeating solitary waves with even spacing over $X\in[-\infty,\infty]$ as in (B1) could give only an approximate solution to the KdV equation is incorrect. Toda's proof was based on the infinite product of the theta function. Reference 26 shows that a more general method of proof is to apply Poisson summation—the same transformation that also generates the Gaussian series of the theta function—directly to the Fourier series of $u(x,t)$ given by (A9) of Ref. 1, and gives similar hyperbolic series for the elliptic functions dn, cn, and sn. The handbook of Gradshteyn and Ryzhik[27] lists some 21 other known Fourier series for various ratios and combinations of elliptic functions, and all can presumably be Poisson summed in the same way.

Unfortunately, the Fourier coefficients for the hyperelliptic functions, i.e., $u(x,t)$ for $N>1$, are not known although the theta function coefficients are known for all N. As a result, the Poisson summation method can only be applied to the theta function except for the special case of the ordinary cnoidal wave. Consequently, the author's earlier comment

that the theta functions provide the only efficient way of generalizing solitary waves to spatially periodic functions remains true for $N > 1$.

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[16]The constant is 12α where $\alpha \equiv R_{11}\,k_1{}^2 + 2R_{12}\,k_1\,k_2 + R_{22}\,k_2{}^2$.
[17]Some care is necessary in interpreting Fig. 3 correctly in terms of sine waves. First, the theta function $\theta\,[{}^0_1](X,Y;\mathbf{T}) \equiv \theta\,[{}^0_0](X+\frac{1}{2}, Y+\frac{1}{2};\mathbf{T})$ is used to generate the graphs; as explained in Appendix A, $\theta\,[{}^0_1]$ is more convenient in the solitary wave regime, but it differs by phase factors from the $\theta\,[{}^0_0]$ which is used everywhere when discussing theta Fourier series. Second, expanding the logarithm of the theta function and then taking the second derivative multiplies all Fourier components by a minus sign. Thus, the "fundamental" referred to in the text is $-\cos[2\pi(X + \frac{1}{2})] = \cos(2\pi X)$. Third, the graphs were made in the [1,1] representation, i.e., $k_1 = k_2 = 1$, which is unnatural for Fourier series as explained in Sec. VI of this work, in Appendix A of Ref. 6, and Sec. VI of Ref. 7. The second harmonic is proportional to $-\cos[2\pi(X + Y + \frac{1}{2} + \frac{1}{2})] = -\cos[2\pi(X + Y)]$. Thus, the fundamental and second harmonic are out of phase at $t = 0$ at $x = 0$ and the fundamental has a peak there, even though naive use of (2.3) would seem to imply both should be negative for $x = t = 0$. I ask the reader's indulgence for this long-winded explanation, but as is the theme of Ref. 7, the need to use different sets of wavenumbers to interpret the double cnoidal wave as sine waves or as solitons sometimes even left the author confused!
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Perturbation series for the double cnoidal wave of the Korteweg–de Vries equation

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(Received 22 March 1983; accepted for publication 22 June 1984)

By means of the theorems proved earlier by the author, the problem of the double cnoidal wave of the Korteweg–de Vries equation is reduced to four algebraic equations in four unknowns. Two of the unknowns are the nonlinear phase speeds c_1 and c_2. Another is a physically irrelevant integration constant. The fourth unknown is the off-diagonal element of the symmetric, 2×2 theta matrix, which in turn gives the explicit coefficients of the Riemann theta function. The double cnoidal wave $u(x,t)$ is then obtained by taking the second x-derivative of the logarithm of the theta function. Two separate forms of these four nonlinear "residual" equations are given. One is obtained from the Fourier series of the theta function and is useful for small wave amplitude. The other is based on the Gaussian series of the theta function and is highly efficient in the large amplitude regime where the double cnoidal wave is the sum of two solitary waves. Both sets of residual equations can be solved via perturbation theory and results are given to fourth order in the Fourier case and second order in the Gaussian case. The Gaussian-based perturbation series has the remarkable property that it converges more and more rapidly as the wave amplitude increases; the zeroth-order solution is the familiar double solitary wave. Numerical comparisons show that the two complementary perturbation series give accurate results in all the important regions of parameter space. (The "unimportant" regions are those in which the double cnoidal wave is an ordinary cnoidal wave subject to a very weak perturbation.) This is turn implies that even for moderate wave amplitude where the nonlinear interactions are not weak, and yet the solitary wave peaks are not well separated, at least to the eye, it is still qualitatively legitimate to describe the double cnoidal wave as either the sum of two sine waves or of two solitary waves of different heights.

PACS numbers: 02.30.Jr, 02.60.Lj, 02.30.Mv

I. INTRODUCTION

In an earlier work, the author[1] discussed the use of theta functions to study the dynamics of "polycnoidal waves," which is the term coined by the author for the spatially periodic solutions of the Korteweg–de Vries (KdV) and other soliton equations. The general theorems proved there, however, were applied only to the simplest case of the 1-polycnoidal wave, i.e., the ordinary cnoidal wave discovered by Korteweg and de Vries in 1895. This paper is the second article in a three part follow-up[2,3] which will apply the earlier results to the double cnoidal wave of the KdV equation. Throught this paper, the term "double cnoidal" will be used interchangeably with "2-polycnoidal" to denote that generalization of the cnoidal wave which is characterized by two distinct phase speeds, amplitudes, and widths.

One major theme of Ref. 1 is that by using the Gaussian series of the theta function for large amplitude waves and the complementary Fourier series for small amplitude waves, one can calculate the single cnoidal wave through perturbation series to very high accuracy for all values of the parameters. In the worst possible case, which is when the two series converge at equal rates, it was shown that the zeroth-order approximations give the phase speed to within 5% relative error while the first-order approximation is accurate to within 0.03%; the approximations for wave shape are similarly accurate. The purpose of this article is to show that one can also obtain good results for the double cnoidal wave by again deriving two complementary perturbation series based on the Gaussian and Fourier representations of the theta function, respectively.

Although the Korteweg–de Vries equation

$$u_t + u\,u_x + u_{xxx} = 0 \tag{1.1}$$

is a partial differential equation, the theta function series for the double cnoidal wave contains only four free parameters: The coefficients of the infinite series for the theta function are completely specified once these four parameters are known. Independently, Boyd[1] and Nakamura[4] were able to show that the problem of finding the double cnoidal solutions of (1.1) can be reduced to solving a system of four algebraic equations for the theta function parameters. This, together with the overlapping of the complementary large amplitude (Gaussian) and small amplitude (Fourier) expansions, makes it possible to derive efficient, accurate perturbation series that describe both the phase speeds and shape of the double cnoidal wave for all possible values of the parameters.

The next section derives these four algebraic equations, the implicit dispersion relation, for both the Fourier and Gaussian expansions. (The Fourier equations can be obtained as a special case of the Gaussian.) Section III discusses the general method of solving a set of nonlinear equations via perturbation theory. Section IV and V give the actual results for the Fourier and Gaussian expansion, respectively. Mixed Fourier–Gaussian series are described briefly in Sec. VI. The errors in these expansions are discussed in Sec. VII. The

 0022-2488/84/123402-13$02.50

paper ends with a final section that summarizes what has gone before and discusses the possibility of extending perturbation theory to other exactly integrable soliton equations.

II. THE RESIDUAL EQUATIONS (IMPLICIT DISPERSION RELATION)

The solution $u(x,t)$ of the KdV equation is related to the theta function via the transformation

$$u = 12(\ln\theta)_{xx}. \tag{2.1}$$

The theta functions themselves satisfy a transformed version of the KdV equation which was first given by Hirota[5] and which will therefore be referred to in what follows as the "Hirota–Korteweg–de Vries" (HKdV) equation. The most compact representation of this bilinear equation is in terms of certain operators introduced by Hirota himself and defined by

$$D_x{}^n D_t{}^m(F\cdot G)\equiv\left[\left(\frac{\partial}{\partial x}-\frac{\partial}{\partial x'}\right)^n\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial t'}\right)^m \times F(x,t)G(x',t')\right]_{\substack{x'=x,\\ t'=t}} \tag{2.2}$$

where the notation indicates that x' and t' are to be replaced by x and t after the differentiation has been performed. The HKdV equation is then

$$(D_x{}^4 + D_xD_t)(\theta\cdot\theta) = 2A\theta^2 \quad [\text{HKdV}], \tag{2.3}$$

where A is a constant of integration which must be determined in the course of solution.

The theta function solutions of (2.3), dubbed "N-polycnoidal" waves in Ref. 1, are functions of the N-dimensional Riemann theta function. The double cnoidal wave, the only example considered here, is the special case $N=2$. The classic theta function notation is discussed in part one of this three part sequence (Ref. 2).

Here it will suffice to note that the "phase" or "angle" variables are defined by

$$X = k_1(x - c_1t) + \phi_1, \tag{2.4}$$

$$Y = k_2(x - c_2t) + \phi_2, \tag{2.5}$$

where the constants k_i, c_i, and ϕ_i are wavenumbers, phase speeds, and phase factors, respectively. Please keep in mind that there is only a single spatial variable x; X and Y are propagating arguments with no direct physical interpretation. Reference 2 describes how to pass from X-Y space to x-t space in more detail.

The Fourier series for the theta function is

$$\theta = \sum_{\substack{n_1=-\infty\\ [\text{integers}]}}^{\infty}\sum_{n_2=-\infty}^{\infty}\exp(-\{T_{11}n_1{}^2 + 2T_{12}n_1n_2 + T_{22}n_2{}^2\}) \times\exp[2\pi i(n_1X + n_2Y)], \tag{2.6}$$

where the sums are taken over all integers including 0. The constants T_{11}, T_{12}, and T_{22} are the elements of the so-called "theta matrix." For simplicity, the notation differs slightly from the usual in that a factor of $i\pi$ has been absorbed into theta matrix elements as explained in Ref. 2.

The complementary Gaussian series is

$$\theta = \sum_{\substack{n_1=-\infty\\ [\text{half-integers}]}}^{\infty}\sum_{n_2=-\infty}^{\infty}\exp\left(-\left\{\left(\frac{R_{11}}{2}\right)(X+n_1)^2 + R_{12}(X+n_1)(Y+n_2) + \left(\frac{R_{22}}{2}\right)(Y+n_2)^2\right\}\right), \tag{2.7}$$

where the sums now range over the half-integers, i.e., $\pm\frac{1}{2}$, $\pm\frac{3}{2}$, $\pm\frac{5}{2}$, etc., instead of over the integers as in the Fourier series (2.6). The 2×2 symmetric matrix whose elements are the constants R_{11}, R_{12}, and R_{22} is loosely called the "inverse theta matrix" since it is proportional to the inverse of the matrix formed from the T_{ij}'s that appear in the Fourier series.[2]

The next step is to simply rewrite the theta series as functions of the physical variables (x,t) using the definitions of (X,Y) given above, substitute the series into the HKdV equation, and collect terms. The resulting sums depend upon how the bilinear operators of the HKdV equation affect a typical pair of terms in the series, so it is useful to define such a pair of terms as

$$F\equiv\exp(-(\alpha/2)x^2 - \beta xt - (\gamma/2)t^2) \times\exp(-[\delta_1n_1 + \delta_2n_2 + \delta_p]x - [\epsilon_1n_1 + \epsilon_2n_2 + \epsilon_p]t), \tag{2.8}$$

$$G\equiv\exp(-(\alpha/2)x^2 - \beta xt - (\gamma/2)t^2) \times\exp(-[\delta_1n_1' + \delta_2n_2' + \delta_p]x - [\epsilon_1n_1' + \epsilon_2n_2' + \epsilon_p]t), \tag{2.9}$$

where the Greek parameters (α,β,γ, and so on) are linear functions of the theta matrix elements, wavenumbers, and phase speeds that will be given explicitly in Sec. V. The forms (2.8) and (2.9) are the natural definitions for the Gaussian series, but they can be specialized to the Fourier series, too, by setting the second-degree exponents α, β, and γ equal to zero and replacing the pseudowavenumbers δ_1 and δ_2 and pseudofrequencies ϵ_1 and ϵ_2 by $2\pi i k_1$, and so on. Thus, it is sufficient to consider the Gaussian case alone. Note that the second-degree exponents are the same for all terms in a given series; only the linear exponents are different and only through the replacement of (n_1,n_2) by (n_1',n_2').

Defining a function zeta via

$$(D_x{}^4 + D_xD_t - 2A)(F\cdot G) \equiv\zeta(n_1 - n_1', n_2 - n_2'; \alpha,\beta,\gamma,\delta_1,\delta_2,\epsilon_1,\epsilon_2,A)FG \tag{2.10}$$

one can use the theorems proved in Sec. VI of Ref. 1 to show that for the HKdV equation,

$$\zeta(m,n,\alpha,\beta,\gamma,\delta_1,\delta_2,\epsilon_1,\epsilon_2,A) = (m\delta_1 + n\delta_2)^4 + (m\delta_1 + n\delta_2)[(\epsilon_1 - 12\alpha\delta_1)m + (\epsilon_2 - 12\alpha\delta_2)n] + 12\alpha^2 - 2\beta - 2A. \tag{2.11}$$

The residual function $\rho(x,t)$, which is defined by

$$\rho(x,t)\equiv(D_x{}^4 + D_xD_t - 2A)(\theta\cdot\theta) \tag{2.12}$$

becomes, after substituting either of the theta series (2.6) or (2.7) into (2.12), invoking (2.10), and collecting terms

$$\rho = \exp(-\alpha x^2 - 2\beta xt - \gamma t^2 - 2\,\delta_p x - 2\epsilon_p t - 2\Phi_p) \text{ (times)}$$
$$\times \sum_{\substack{j=-\infty \\ [\text{integers}]}}^{\infty} \sum_{k=-\infty}^{\infty} \rho_{jk} \exp(-[\delta_1 j + \delta_2 k]x$$
$$-[\epsilon_1 j + \epsilon_2 k]t - [\Phi_1 j + \Phi_2 k]), \tag{2.13}$$

where both sums are taken over the integers for either the Gaussian or Fourier theta series.

A theta series is a solution of the HKdV equation if and only if $\rho(x,t) \equiv 0$. Since the terms in (2.13) are linearly independent, this in turn implies that

$$\rho_{jk} = 0, \quad j = 0,1,2,..., \quad k = 0,1,2,..., \tag{2.14}$$

for all integers j and k. Thus, by substituting an infinite series into the differential equation, one reduces it to an infinite set of coupled algebraic equations which determine the coefficients of the series.

Since the theta function is uniquely determined by a finite number of parameters (the three theta matrix elements plus the wavenumbers and phase speeds), one seems to have a problem: infinitely more equations than unknowns! Independently, Boyd[1] and Nakamura[4] resolved this apparent paradox by proving that only four of the infinite set of "residual equations" (2.14) are independent: the rest are proportional to the chosen four, which may be conveniently taken as $j = 0,1$ and $k = 0,1$.

The goal of this paper is simply to solve these four algebraic equations via perturbation theory.

III. PERTURBATION THEORY FOR GENERAL SYSTEMS OF ALGEBRAIC EQUATIONS

Suppose one is given a system of N algebraic equations in N unknowns which depend upon a small parameter,

$$F_i(x_1,x_2,...,x_N;\epsilon) = 0, \quad i = 1,2,...,N, \tag{3.1}$$

such that a solution $\mathbf{x}^{(0)} = (x_1^{(0)},x_2^{(0)},...,x_N^{(0)})$ is known for $\epsilon = 0$. A regular perturbation expansion in ϵ can be calculated through the following three steps: (i) expand each F_i as a power series in the $N+1$ small variables $([x_1 - x_1^{(0)}], [x_2 - x_2^{(0)}],...,[x_N - x_N^{(0)}];\epsilon)$; (ii) expand each of the unknowns $(x_1,x_2,...,x_N)$ as a power series in ϵ, substitute in the series obtained in the first step and collect powers in ϵ; (iii) order-by-order in ϵ, solve the equations that result from demanding that the expansions for each F_i obtained in the second step are identically equal to 0.

If one writes

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} = \mathbf{x}^{(0)} + \epsilon\mathbf{x}^{(1)} + \epsilon^2\mathbf{x}^{(2)} + \cdots, \tag{3.2}$$

then

$$\mathbf{J}\mathbf{x}^{(N)} = \mathbf{F}^{(N)}(\mathbf{x}^{(0)},\mathbf{x}^{(1)},...,\mathbf{x}^{(N-1)};\epsilon), \tag{3.3}$$

where $\mathbf{F}^{(N)}$ is the column vector whose elements are those terms at $O(\epsilon^N)$ in the power series of F_i which depend only on the lower-order coefficients in the series in the unknowns ($\mathbf{x}^{(0)}$ and so on) which have already been calculated where $\mathbf{J}$ denotes the usual $N \times N$ Jacobian matrix of the functions F_i, evaluated at $\epsilon = 0$. The elements J_{ij} of J are

$$J_{ij} \equiv \frac{\partial F_i}{\partial x_j}(\mathbf{x}^{(0)};0). \tag{3.4}$$

If the equations F_i are polynomials[6] in the unknowns, then calculating the right-hand side of (3.3) is merely a matter of rearranging power series. Since it is always possible to solve a system of linear equations like (3.3)— a matrix equation is one of the types that is always solvable—the only delicate part of the business is calculating the lowest-order solution $\mathbf{x}^{(0)}$, since this may involve solving nonlinear equations. Fortunately, in the important cases for the double cnoidal wave, solving the zeroth-order perturbation equations is easy.

Although routine, the power series rearrangements and algebra needed to repeatedly compute and then solve (3.3) quickly becomes laborious as the perturbation order increases. The perturbation series were therefore calculated using the algebraic manipulation language REDUCE 2, which can add, multiply, differentiate, and collect terms in polynomials of several variables in symbolic form without requiring the substitution of numerical values as in FORTRAN. Regular (as opposed to singular) perturbation theory is ideally suited to REDUCE 2 and vice versa: The program to compute each of the perturbation series given in the next two sections had fewer than 50 executable statements (!) and cost of the final runs was less than $10.00.

A special advantage of employing an algebraic manipulation language is that different soliton equations in the same class as the KdV differ only in the function ζ defined in Sec. II. Therefore, perturbation series for the Boussinesq water wave equation and several others can be obtained by rerunning the program after modifying only a couple of statements.

A second advantage is that the computer can substitute the perturbation series back into the original nonlinear equations to verify that the solution has indeed been calculated correctly.

The same algorithm, and very nearly the same computer program, can also be applied to higher polycnoidal waves. The major difference is that for the triple cnoidal wave, for example, which is the generalization of three sine waves (small amplitude) and three solitons (large amplitude), $N = 7$ instead of 4, and the series are more complicated because of the greater number of parameters.

IV. SMALL AMPLITUDE (FOURIER SERIES) PERTURBATION THEORY

As noted earlier, the residual equations that determine the theta function Fourier series are a special case of the corresponding more general expressions for the Gaussian series theory. Making the replacements $\delta_i \to 2\pi i k_i$, $\epsilon_i \to -2\pi_i k_i c_i$ and $\alpha = \beta = \gamma = 0$, one finds

$$\rho_{jk} = \sum_{\substack{n_1=-\infty \\ [\text{integers}]}}^{\infty} \sum_{n_2=-\infty}^{\infty} q_1^{n_1^2 + (n_1 - j)^2} q_2^{n_2^2 + (n_2 - k)^2}$$
$$\times e^{-2T_{12}[n_1 n_2 + (n_1 - j)(n_2 - k)]}$$
$$\times \zeta(2n_1 - j, 2n_2 - k; k_1,k_2,c_1,c_2,A), \tag{4.1}$$

where

$$\zeta(m,n;k_1,k_2,c_1,c_2,A)\equiv 16\pi^4(k_1m+k_2n)^4+4\pi^2(k_1m+k_2n)\times(k_1c_1m+k_2c_2n)-2A, \tag{4.2}$$

$$q_i\equiv e^{-T_{ii}}\ [\text{"nomes"}]. \tag{4.3}$$

The four equations to be solved are

$$\rho_{jk}=0,\quad j=0,1;\quad k=0,1. \tag{4.4}$$

The input parameters are the wavenumbers (k_1,k_2) and either the diagonal theta matrix elements $(T_{11},\ T_{22})$ or the nomes (q_1,q_2). The perturbation series given here are power series in ${q_1}^2$ and ${q_2}^2$. The nomes (or equivalently, T_{11} and T_{22}) determine the amplitudes of the two sine waves that form the lowest-order approximation, while k_1 and k_2 are the wavenumbers of these two waves.

The four unknowns whose column vector is **x** are the two phase speeds (c_1,c_2), the constant of integration A for the HKdV equation (which has no physical significance), and the exponential of the off-diagonal theta matrix element

$$\begin{pmatrix}x_1\\x_2\\x_3\\x_4\end{pmatrix}=\begin{pmatrix}c_1\\c_2\\A\\e^{-2T_{12}}\end{pmatrix}. \tag{4.5}$$

Novikov[7] has stressed that double cnoidal waves may be almost periodic in space as well as in time. In other words, the ratio of k_1/k_2 is mathematically arbitrary and may even be irrational. Therefore, it is useful to first give the general solution for symbolic k_1 and k_2 [to $O({q_1}^4,{q_2}^4)$] and then the special $k_1=1$, $k_2=2$ solution to $O({q_1}^8,{q_2}^8)$.

$$c_1=-{k_1}^2(1-24{q_1}^2-72{q_1}^4)+384{q_2}^4{k_2}^6/([{k_1}^2-{k_2}^2]^2), \tag{4.6}$$

$$c_2=-{k_2}^2(1-24{q_2}^2-72{q_2}^4)+384{q_1}^4{k_1}^6/([{k_1}^2-{k_2}^2]^2), \tag{4.7}$$

$$A=0+12({k_1}^4{q_1}^2+{k_2}^4{q_2}^2)+72({k_1}^4{q_1}^4+{k_2}^4{q_2}^4)-768{q_1}^2{q_2}^2{k_1}^4{k_2}^4/([{k_1}^2-{k_2}^2]^2), \tag{4.8}$$

$$\begin{aligned}e^{-T_{12}}=&\{[(k_1-k_2)/(k_1+k_2)]^2\}\\&+32k_1k_2\{({k_1}^2{q_1}^2+{k_2}^2{q_2}^2)/[(k_1+k_2)^4]\}\\&+32k_1k_2\{{k_1}^2{q_1}^4(-9{k_1}^4+16{k_1}^3k_2\\&-18{k_1}^2{k_2}^2+3{k_2}^4)+{k_2}^2{q_2}^4(3{k_1}^4-18{k_1}^2{k_2}^2\\&+16k_1{k_2}^3-9{k_2}^4)+16{k_1}^2{k_2}^2{q_1}^2{q_2}^2(-3{k_1}^2\\&+2k_1k_2-3{k_2}^2)\}/[(k_1+k_2)^4({k_1}^2-{k_2}^2)^2].\end{aligned} \tag{4.9}$$

The special solution for a wave and its second harmonic $(k_1=1,\ k_2=2)$ is

$$\begin{aligned}c_1=4\pi^2\{&-1+24{q_1}^2+72{q_1}^4+(\tfrac{8\,192}{3}){q_2}^4\\&+96{q_1}^6-32(63\,488{q_2}^6+69\,632{q_1}^2{q_2}^4)/27\\&+168{q_1}^8+114\,688(3\,064{q_1}^4{q_2}^4+16\,704{q_1}^2{q_2}^6\\&+6\,025{q_2}^8)/243\},\end{aligned} \tag{4.10}$$

$$\begin{aligned}c_2=16\pi^2\{&-1+24{q_2}^2+72{q_2}^4+(\tfrac{32}{3}){q_1}^4\\&+96{q_2}^6-256({q_1}^6+184{q_1}^4{q_2}^2)/27\\&+168{q_2}^8+64(535{q_1}^8+104\,448{q_1}^6{q_2}^2\\&+658\,528{q_1}^4{q_2}^4)/243\},\end{aligned} \tag{4.11}$$

$$\begin{aligned}A=0+16\pi^4\{&12{q_1}^2+192{q_2}^2\\&+72{q_1}^4+1\,152{q_2}^4-(\tfrac{4\,096}{3}){q_1}^2{q_2}^2\\&+144{q_1}^6+2304{q_2}^6\\&+204\,800({q_1}^4{q_2}^2+13{q_1}^2{q_2}^4)/27\\&+336{q_1}^8+5376{q_2}^8-16\,384(495{q_1}^6{q_2}^2\\&+38\,461{q_1}^4{q_2}^4+89\,475{q_1}^2{q_2}^6)/243\},\end{aligned} \tag{4.12}$$

$$\begin{aligned}e^{-T_{12}}=&(\tfrac{1}{9})+(\tfrac{64}{81}){q_1}^2+(\tfrac{256}{81}){q_2}^2\\&-(\tfrac{64}{729})[{q_1}^4+340{q_2}^4+704{q_1}^2{q_2}^2]\\&+256[19\,972{q_2}^6+93\,168{q_1}^2{q_2}^4\\&+19\,728{q_1}^4{q_2}^2+37{q_1}^6]/6\,561\\&-(\tfrac{30\,994\,432}{243}){q_1}^4{q_2}^4\\&-(\tfrac{64}{19\,683})(2\,887{q_1}^8+8\,816\,428{q_2}^8)\\&-(\tfrac{16\,384}{59\,049})(29\,029{q_1}^6{q_2}^2+736\,867{q_1}^2{q_2}^6).\end{aligned} \tag{4.13}$$

Several features of these expansions deserve comment. First, the numerical coefficients are rather large for high order, suggesting that the range of accuracy in the q_1-q_2 plane is too small to be useful. To show that this is not true, contours of constant error for the perturbation series of various orders are given in Figs. 1 and 2 in Sec. VII.

Second, the expansions proceed in powers of ${q_1}^2(=\exp[-2T_{11}])$ and ${q_2}^2(=\exp[-2T_{22}])$ rather than q_1 and q_2 themselves even though the series for the theta functions have coefficients that are power series in the unsquared variables q_1 and q_2. This obviously improves the accuracy and usefulness of the perturbation series.

Third, the perturbation series are sparse not merely because all the odd powers vanish but because some of the expected even powers are missing, too. The series for c_1, for example, has zero coefficients for ${q_2}^2$, ${q_1}^2{q_2}^2$, ${q_1}^4{q_2}^2$, and ${q_1}^6{q_2}^2$, i.e., one missing term at each order so that the series through $O({q_1}^8,{q_2}^8)$ contains only eleven terms. Similar sparsity exists for the other quantities.

Fourth, although the series for A has been listed for completeness (one cannot solve for the other unknowns without simultaneously obtaining A, too) A is only the constant of integration for the Hirota–Korteweg–deVries equation and has no direct physical significance. It is never necessary to evaluate A to compute the double cnoidal wave solutions of the KdV equation itself.

Fifth and most important, although $u(x,t)$, the KdV solution, is defined in terms of an infinite series, it is never necessary to explicitly tabulate the coefficients of the series. Instead the three dependent parameters T_{12}, c_1, and c_2 together with the four free parameters T_{11}, T_{22}, k_1, and k_2 completely determine all the coefficients of the theta Fourier series (2.6), which in turn determines $u(x,t)$ via (2.1)

Ordinary Stokes' expansions, obtained via the method of multiple scales as in Appendix B of Ref. 1, can be calculated for almost any wave equation, but each Fourier component—and their numbers grow as the square of the perturbation order—must be calculated through a separate expansion as complicated as that for the phase speeds c_1 and

c_2. To need only three perturbation series instead of many is thus a great simplification.

V. LARGE AMPLITUDE (GAUSSIAN SERIES) PERTURBATION THEORY

For large amplitude, the double cnoidal wave problem reduces to solving the four simultaneous nonlinear residual equations $\rho_{jk}=0$, where the residuals are given by the Gaussian series

$$\rho_{jk}=\sum_{\substack{n_1=-\infty \\ [\text{half-integers}]}}^{\infty}\sum_{\substack{n_2=-\infty \\ [\text{half-integers}]}}^{\infty} q_1'^{n_1^2+(n_1-j)^2} q_2'^{n_2^2+(n_2-k)^2} \times\exp(-R_{12}\{n_1n_2+(n_1-j)(n_2-k)\}) \times\zeta(2n_1-j,2n_2-k;\alpha,\beta,\gamma,\delta_1,\delta_2,\epsilon_1,\epsilon_2,A), \quad j=0,1 \;\; k=0,1, \tag{5.1}$$

where

$$q_i'\equiv e^{-R_{ii}/2} \quad [\text{"complementary nomes"}]. \tag{5.2}$$

Equation (5.1) is very similar in form to its Fourier series counterpart, (4.1), but there are some noteworthy differences. As indicated in the square brackets under the summation symbols, the sums do not run over the integers but rather over the "half-integers" $\pm\frac{1}{2}$, $\pm\frac{3}{2}$, $\pm\frac{5}{2}$,.... The "nomes" q_1 and q_2 are replaced by the "complementary nomes" q_1' and q_2' which are defined in terms of the elements of the inverse theta matrix. A factor 2 is present in (5.2) which is missing from (4.2) and the factor of 2 multiplying T_{12} in (4.1) has no counterpart in the coefficient of R_{12} in (5.1).

The major difference is in the form of ζ which is

$$\zeta(m,n;\alpha,\beta,\gamma,\delta_1,\delta_2,\epsilon_1,\epsilon_2,A) =(\delta_1 m+\delta_2 n)^4+(\delta_1 m+\delta_2 n)[(\epsilon_1-12\alpha\delta_1)m +(\epsilon_2-12\alpha\delta_2)n]+12\alpha^2-2\beta-2A, \tag{5.3}$$

where the parameters are related to the wavenumbers and phase speeds via

$$\alpha=R_{11}k_1^2+2R_{12}k_1k_2+R_{22}k_2^2, \tag{5.4}$$

$$\beta=-R_{11}k_1^2c_1-R_{12}k_1k_2(c_1+c_2)-R_{22}k_2^2c_2, \tag{5.5}$$

$$\gamma=R_{11}k_1^2c_1^2+2R_{12}k_1k_2c_1c_2+R_{22}k_2^2c_2^2, \tag{5.6}$$

$$\delta_1=R_{11}k_1+R_{12}k_2, \tag{5.7}$$

$$\delta_2=R_{12}k_1+R_{22}k_2, \tag{5.8}$$

$$\epsilon_1=-R_{11}k_1c_1-R_{12}k_2c_2, \tag{5.9}$$

$$\epsilon_2=-R_{12}k_1c_1-R_{22}k_2c_2. \tag{5.10}$$

The parameters δ_1 and δ_2 may be named "pseudowavenumbers" because, as shown in Appendix B, they give the widths of the two solitary waves in the large amplitude, near-soliton regime in the same way that the wavenumbers k_1 and k_2 give the widths of the two sine waves in the small amplitude regime. Similarly, ϵ_1 and ϵ_2 may be labeled "pseudofrequencies" in the sense that $(-\epsilon_1/\delta_1)$ and $(-\epsilon_2/\delta_2)$ are the phase speeds of the two solitary waves for large wave amplitude.

The major complication posed by (5.4)–(5.10) is that the parameters denoted by Greek letters are functions of R_{12}, which is one of the unknowns. Thus, it is not possible to evaluate any of these parameters *a priori*; instead, one must solve for them as part of the task of solving the residual equations, which would seem to leave us facing an algebraic problem of ghastly complexity.

Fortunately, the situation is not quite as bad as it looks. The function ζ is independent of γ, which is automatically eliminated from $u(x,t)$ by taking the second logarithmic derivative with respect to x. Thus, although γ is needed to graph the theta function, it is quite irrelevant both to solving the residual equations and to evaluating the solution of the Korteweg–de Vries equation, so γ will be ignored in the rest of the discussion.

The parameter β appears in ζ only as the sum $\beta+A$. Thus, if β is artificially set equal to 0 to reduce the number of unknowns, the solution of the residual equation will be unchanged except for A, but A has no physical significance. Therefore, the calculations presented will be done with $\beta=0$; after R_{12} and the other unknowns have been determined, one can then evaluate β and add the result to the computed A to obtain a final solution which is completely consistent with the original equations (5.1)–(5.10).

The parameter α has a slightly more complex role. One can easily show from (5.3), (5.9), (5.10), (2.1), and (2.9) that the results of a calculation in which α is artificially set equal to 0 differ from those in which α is retained via

$$A\,[\text{with }\alpha]=A(\alpha=0)+6\alpha^2, \tag{5.11}$$

$$c_1[\text{with }\alpha]=c_1(\alpha=0)-12\alpha, \tag{5.12a}$$

$$c_2[\text{with }\alpha]=c_2(\alpha=0)-12\alpha, \tag{5.12b}$$

$$u(x,t)[\text{with }\alpha]=-12\alpha+u(x+12\alpha t,t), \quad (\alpha=0). \tag{5.13}$$

Since A has no physical significance, the important role of α is to add a constant to $u(x,t)$ while simultaneously increasing all the phase speeds of the "angle" variables by the same constant. As noted in Ref. 2, the theta function solution of the Korteweg–de Vries equation is that solution which has $\langle u\rangle=0$, where $\langle\ \rangle$ denotes an average over the periodicity interval. In the near-soliton regime, this is awkward because it implies that the solitons asymptote to $u=-12\alpha$ instead of to $u=0$, which is the usual asymptotic solution as $|x|\to\infty$ in the spatially unbounded problem. Setting $\alpha=0$ merely causes the solitons to asymptote to 0.[8] Thus, the parameter α is no real trouble either.

Difficulties with the "pseudofrequencies" ϵ_1 and ϵ_2 can be avoided by simply taking them as unknowns in the residual equations. After ϵ_1, ϵ_2, and R_{12} have been obtained by solving the rest of the problems, c_1 and c_2 can be obtained by solving (5.9) and (5.10) as a pair of linear equations in two unknowns. Alternatively, one could use (5.9) and (5.10) directly in ζ to replace ϵ_1 and ϵ_2 wherever they appeared by expressions in c_1, c_2, and R_{12}, which are the usual unknowns of the residual equations, but this makes the ρ_{jk} much more complicated, so it is far less work to consider ϵ_1 and ϵ_2 as the unknowns and then compute c_1 and c_2 at the end.

Unfortunately, there is little one can do with the two remaining parameters, the "pseudowavenumbers" δ_1 and δ_2. The simplest set of algebraic nonlinear equations one can solve simultaneously is the set of six equations in the unknowns (A, R_{12}, ϵ_1, ϵ_2, δ_1, δ_2): the four residual equations

$\rho_{jk} = 0$ plus the pair of equations which define δ_1 and δ_2, (5.7) and (5.8). However, the rather special form of these equations—(5.7) and (5.8) involve only three of the six unknowns—means that it is not necessary to solve all six equations simultaneously. Instead, one can pretend that δ_1 and δ_2 are independent free parameters and solve the four residual equations via perturbation theory exactly as for the Fourier series case in the preceding section. Adding two new parameters to the four that already exist (R_{11}, R_{22}, k_1, k_2) would seem to greatly complicate the chore of solving $\rho_{jk} = 0$, but it actually does not because k_1 and k_2 do not appear explicitly in the Gaussian form of ζ (5.3). Instead, δ_1 and δ_2 appear in place of the wavenumbers in the analogous terms of ζ. Thus, this device of pretending δ_1 and δ_2 are independent parameters leads to solutions of the coupled set $\rho_{jk} = 0$ which are neither more nor less complicated than the analogous solution in the Fourier case for general k_1 and k_2. Just as the Fourier solution for general k_1 and k_2 (as opposed to $k_2 = 2k_1$) was taken only up to and including second order $[O(q_1^4, q_2^4)]$, so also the Gaussian solution of the residual equations will only be carried to second order also.

The residual equations (implicit dispersion relation) are defined by infinite series; to calculate the solution to a given order, it is sufficient to truncate the series of ρ_{jk} after this same order. The truncated residual series in the Fourier case was omitted from the previous section because it is given (to lowest order) in Appendix A, but it is useful to give the series to second order for at least one of the two cases so that the reader can see more clearly what must be solved. The series have been simplified by exploiting the general symmetry relation (true in Fourier case also)

$$\zeta(m,n) = \zeta(-m,-n) \quad \text{for all } m,n, \tag{5.14}$$

and by dividing out common factors, which is why equal signs have been replaced by proportionality symbols. In addition

$$\chi \equiv e^{-R_{12}} \tag{5.15}$$

has been used to replace appearances of R_{12} so as to make the series rational in all parameters and unknowns.

$$\rho_{00} \propto \zeta(1,1)\chi + \zeta(1,-1) + q_1'^4[\zeta(3,1)\chi^2 + \zeta(3,-1)/\chi] + q_2'^4[\zeta(1,3)\chi^2 + \zeta(1,-3)/\chi], \tag{5.16}$$

$$\rho_{10} \propto \zeta(0,1) + q_1'^2[\zeta(2,1)\chi + \zeta(2,-1)/\chi] + q_2'^4\zeta(0,3), \tag{5.17}$$

$$\rho_{01} \propto \zeta(1,0) + q_2'^2[\zeta(1,2)\chi + \zeta(1,-2)/\chi] + q_1'^4\zeta(3,0), \tag{5.18}$$

$$\rho_{11} \propto \zeta(0,0) + 2[q_1'^2\zeta(2,0) + q_2'^2\zeta(0,2)] + 2q_1'^2q_2'^2[\zeta(2,2)\chi^2 + \zeta(2,-2)/\chi^2]. \tag{5.19}$$

These rather innocent-looking expressions, (5.16)–(5.19), become exceedingly messy when $\zeta(m,n)$ is evaluated according to (5.3), so they were solved perturbatively using the algebraic manipulation language REDUCE 2 to perform (and check!) the algebra. Note that these series, like their solutions and the Fourier perturbation series given in Sec. IV, are "sparse": many expected terms in the series are identically equal to 0. Equation (5.16), for example, contains no first-order terms at all, and only five of the possible 12 second-order terms appear in the set.

The corresponding solutions are given below. Note that the parameters α and β have been inserted in the proper places so that the results are fully consistent with (5.3)

$$\epsilon_1 = \delta_1(12\alpha - \delta_1^2) + 24q_1'^2\delta_1^3 + 24\delta_1[3q_1'^4(\delta_1^2\delta_2^4 - 2\delta_1^4\delta_2^2 + \delta_1^6) + 16q_2'^4\delta_2^6]/[(\delta_2^2 - \delta_1^2)^2], \tag{5.20}$$

$$\epsilon_2 = \delta_2(12\alpha - \delta_2^2) + 24q_2'^2\delta_2^3 + 24\delta_2[16q_1'^4\delta_1^6 + 3q_2'^4(\delta_2^6 - 2\delta_1^2\delta_2^4 + \delta_1^4\delta_2^2)]/[(\delta_2^2 - \delta_1^2)^2], \tag{5.21}$$

$$A = 6\alpha^2 - \beta + 12q_1'^2\delta_1^4 + 12q_2'^2\delta_2^4 + 24[3q_1'^4(\delta_1^4\delta_2^4 - 2\delta_1^6\delta_2^2 + \delta_1^8) - 32q_1'^2q_2'^2\delta_1^4\delta_2^4 + 3q_2'^4(\delta_2^8 - 2\delta_1^2\delta_2^6 + \delta_1^4\delta_2^4)]/[(\delta_2^2 - \delta_1^2)^2], \tag{5.22}$$

$$e^{-R_{12}} = (\delta_1 - \delta_2)^2/(\delta_1 + \delta_2)^2 + 32\delta_1\delta_2(q_1'^2\delta_1^2 + q_2'^2\delta_2^2)/(\delta_1 + \delta_2)^4 + 32\delta_1\delta_2[(q_1'^4(3\delta_1^2\delta_2^4 - 18\delta_1^4\delta_2^2 + 16\delta_1^5\delta_2 - 9\delta_1^6) - q_1'^2q_2'^2(48\delta_1^2\delta_2^4 - 32\delta_1^3\delta_2^3 + 48\delta_1^4\delta_2^2) + q_2'^4(-9\delta_2^6 + 16\delta_1\delta_2^5 - 18\delta_1^2\delta_2^4 + 3\delta_1^4\delta_2^2)]/[(\delta_1 + \delta_2)^6(\delta_1 - \delta_2)^2]. \tag{5.23}$$

As explained before, δ_1 and δ_2 are not really independent parameters but rather are determined by R_{11} and R_{22} (or equivalently, by q_1' and q_2') through (5.7) and (5.8). It is therefore necessary to solve the triplet system of (5.23) plus (5.7) and (5.8) for the three unknowns (δ_1, δ_2, R_{12}) to obtain a completely consistent solution. However, in the large amplitude regime, δ_1 and δ_2 have a physical interpretation as giving the widths and speeds of the two solitons,

$$u(x,t) \doteq 3\delta_1^2\,\mathrm{sech}^2[(\delta_1/2)(x - \delta_1^2 t + \phi_1)] + 3\delta_2^2\,\mathrm{sech}^2[(\delta_1/2)(x - \delta_2^2 t + \phi_2)], \tag{5.24}$$

where ϕ_1 and ϕ_2 are phase constants at those times when the two solitons are well separated. In the large amplitude regime, $R_{12} \ll R_{11}$, R_{22} so that one has approximately

$$R_{ii} = \delta_i/k_i, \quad i = 1,2. \tag{5.25}$$

Under these circumstances, it may be preferable to take the pseudowavenumbers δ_1 and δ_2 as independent parameters, estimate R_{11} and R_{22} and therefore, q_1' and q_2' via (5.25) and (5.2), and then use (5.20) to (5.23) directly to estimate the importance of the corrections due to spatial periodicity to the lowest-order solution, which is just the spatially unbounded double soliton.[9]

Unfortunately, this crude estimation is all that can be done directly because the lowest-order problem for (5.7), (5.8), and (5.23), which is

$$e^{-R_{12}} = (\delta_1 - \delta_2)^2/(\delta_1 + \delta_2)^2, \tag{5.26}$$

$$\delta_1 = k_1R_{11} + k_2R_{12}, \tag{5.7 bis}$$

$$\delta_2 = k_1 R_{12} + k_2 R_{22}, \tag{5.8 bis}$$

has no closed form solution. It is easy to solve this set numerically, however.

To proceed to higher order, it is convenient to replace δ_1 and δ_2 by

$$\overline{S} \equiv \delta_1 + \delta_2, \tag{5.27}$$

$$\overline{D} \equiv \delta_1 - \delta_2. \tag{5.28}$$

There are two motives for this trick. One is the δ_1 and δ_2 often appear in (5.23) as their sum or difference rather than alone. A second reason is that for the special case of $k_1 = k_2$ (the principal branch or mode of the double cnoidal wave as explained in Ref. 2) the difference variable D is given exactly by the lowest-order solution. In terms of the new variables, the problem becomes (5.23) plus

$$\overline{S} = k_1 R_{11} + k_2 R_{22} + (k_1 + k_2) R_{12}, \tag{5.29}$$

$$\overline{D} = k_1 R_{11} - k_2 R_{22} + (k_2 - k_1) R_{12}. \tag{5.30}$$

The general solution to first order for arbitrary k_1 and k_2 is

$$\overline{S} = S - \Psi(k_1 + k_2), \tag{5.31}$$

$$\overline{D} = D - \Psi(k_2 - k_1), \tag{5.32}$$

$$e^{-R_{12}} = \chi(1 + \Psi), \tag{5.33}$$

where S, D, and χ are the solutions of the lowest-order set

$$S = k_1 R_{11} + k_2 R_{22} - (k_1 + k_2)\ln(\chi), \tag{5.34}$$

$$D = k_1 R_{11} - k_2 R_{22} + (k_1 - k_2)\ln(\chi), \tag{5.35}$$

$$\chi = D^2/S^2, \tag{5.36}$$

[which is equivalent to (5.26) plus (5.7) and (5.8)] and where

$$\Psi = 2(S+D)(S-D)[q_1'^2(S+D)^2 + q_2'^2(S-D)^2]/ \{\chi S^4 - SD^4[k_1(S+D) - k_2(S-D)]/2\}. \tag{5.37}$$

The second-order solution for the special case $k_1 = k_2 = 1$ is

$$\overline{D} = D, \tag{5.38a}$$

$$\overline{S} = S - 2\Psi + \{-32D^4\Psi(q_1'^2 + q_2'^2) + 48D^3S\Psi(q_2'^2 - q_1'^2) + 16DS^3\Psi(q_1'^2 - q_2'^2) + \Psi^2(24D^2S - \chi S^5) + 2S^5 v\}/(S^2[4D^2 - \chi S^3]), \tag{5.38b}$$

$$e^{-R_{12}} = \chi(1 + \Psi) + \{16D^4\Psi(q_1'^2 + q_2'^2) + 24D^3S\Psi(q_1'^2 - q_2'^2) + 8DS^3\Psi(q_2'^2 - q_1'^2) + 2D^2S\Psi^2(S - 6) - S^5 v\}/(S^2[4D^2 - \chi S^3]), \tag{5.39}$$

where as before S, D, and χ are the lowest-order solutions for $(\delta_1 + \delta_2)$, $(\delta_1 - \delta_2)$, and $\exp(-R_{12})$, Ψ is given by (5.37) and

$$v \equiv \{-q_1'^4[S^4 + 2S^3D + 10SD^3 + 5D^4](S+D)^3(S-D) - 8q_1'^2q_2'^2[S^2 + 2D^2](S+D)^3(S-D)^3 - q_2'^4[S^4 - 2S^3D - 10SD^3 + 5D^4](S-D)^3(S+D)\}/(D^2S^6). \tag{5.40}$$

It goes almost without saying that the Gaussian perturbation theory is more cumbersome than its Fourier counterpart at the same; particularly annoying is the necessity of solving the lowest-order set (5.26) plus (5.7)–(5.8) numerically, even though a simple Newton's iteration initialized with $R_{12} = 0$ always seems to work. However, the Gaussian series is that oddity: a perturbation series that converges more and more rapidly as the wave amplitudes becomes larger, so it is an essential component of any complete treatment of polycnoidal waves.

VI. PERTURBED SINGLE-SOLITON REGIMES

The perturbation series derived in the previous two sections were based on the implicit assumption that both diagonal theta matrix elements T_{11} and T_{22} are either very large (Fourier series) or very small (Gaussian series). When one diagonal theta matrix element is very large and the other is very small, however, neither the Fourier series nor the Gaussian series for the theta function converges rapidly as is obvious from inspecting the form of these series.

In Ref. 1, it is shown through numerical examples that these regimes correspond to a single solitary wave slightly perturbed by a small amplitude sine wave, so these parametric neighborhoods are much less interesting than those in which the waves have amplitudes of the same order of magnitude and one or the other of the series given in the previous sections is rapidly convergent. When ($k_1 = 1$ and $k_2 = 2$)

$$T_{11} \ll \pi, \quad T_{22} \gg \pi, \tag{6.1}$$

the solitary wave is of unit period with a height and width determined solely by the magnitude of T_{11}, and the perturbation is of wavenumber 2, i.e., periodic with a period of $\frac{1}{2}$, with a small amplitude roughly equal to $4\exp(-T_{22})$. After the application of a modular transformation[3] to $k_1 = k_2 = 1$, this same regime is found to be characterized by either

$$R_{11} \ll 2\pi, \quad R_{22} \gg \pi, \tag{6.2}$$

or equivalently (since the wavenumbers after the modular transformation are identical) by (6.2) with the direction of the inequalities reversed.

The other perturbed-one-soliton regime occurs when

$$T_{11} \gg \pi, \quad T_{22} \ll \pi. \tag{6.3}$$

The large amplitude component is now of wavenumber 2, so that tall, narrow solitary wave is repeated with half unit period while the small amplitude perturbation is a subharmonic of period one. When the modular transformation is applied to convert to a representation with equal wavenumbers, $k_1 = k_2 = 1$, one finds that the equivalent neighborhood in terms of the inverse theta matrix elements lies around the diagonal in the $R_{11} - R_{12}$ plane,

$$R_{11} \simeq R_{12}. \tag{6.4}$$

The reason for this somewhat surprising result is that the wavenumbers are equal in the $R_{11} - R_{12}$ plane and therefore the roles of the two diagonal inverse theta matrix elements are physically interchangeable and the phase speeds, etc., must be symmetric functions of R_{11} and R_{22}. This implies that the whole of the $T_{11} - T_{22}$ plane must map into the wedge-shaped half of the $R_{11} - R_{22}$ plane which lies below the diagonal (6.4).

The Poisson summation method which was used to

generate the Gaussian series from the theta Fourier series can be applied selectively to just one of the sum variables, either n_1 or n_2, in the infinite series that define the residual function ρ_{ij} (4.1). This is not the most efficient way to proceed because it causes "theta matrix-halving" as explained on p. 384 of Ref. 1, but it shows that in principle, Poisson summation can be applied to generate rapidly converging residual function series (and perturbation series derived from them) in any region of parameter space for polycnoidal waves of any genus N.

A procedure that gives more rapidly converging series is to apply partial Poisson summation directly to the multidimensional theta function and substitute the result into the Hirota–Korteweg–de Vries equation. Shirfuji[10] actually applied this idea to the double cnoidal wave of the Toda lattice problem in 1976, but the independent derivation of the residual equations by Nakamura and Boyd lay in the future, and such results as he obtained came directly from the governing equations of the Toda lattice, and not from Hirota's transformed Toda equation. The theta function can be written as

$$\theta = \theta_4(X) + e^{-T_{22}}\{\theta_4[X - (i/\pi)T_{12}]e^{2\pi iY} + \theta_4[X + (i/\pi)T_{12}]e^{-2\pi iY}\}, \tag{6.5}$$

when $T_{11} \ll T_{22}$, where $\theta_4(X)$ is the usual one-dimensional theta function. Representing θ_4 by its Gaussian series representation [note that (6.5) contains the lowest terms of the Fourier series in the other angle variable Y with higher terms eliminated because of the extreme smallness of $\exp(-T_{22})$] one can substitute (6.5) into the Hirota–Korteweg–de Vries equation and then use the calculus of Hirota operators developed in Ref. 1 to obtain infinite series for the residual equations.

Unfortunately, the resulting zeroth-order approximation is a quartic equation in $\exp(-T_{12})$ and cannot be solved in closed form, unlike its counterpart for the pure Fourier series representation given in Sec. IV. It follows that one is forced to resort to numerical methods even to compute the zeroth-order solution, so this kind of special treatment for the perturbed-one-soliton regimes is not very useful. In the first place, the double cnoidal wave is much more interesting when it is truly a double soliton or a double sine wave than when it is merely a perturbed ordinary cnoidal wave. In the second place, numerical solution of the "pure" Fourier or Gaussian residual equations (4.1) and (4.2) is quick and efficient unless the difference between the magnitudes of the diagonal theta matrix elements is very large, but in that case, the perturbation of the single soliton is very, very small, and therefore uninteresting.

For this reason, no further details will be given about partial Poisson summation of Shirafuji's approximation. For most purposes, the perturbation series derived in the preceding two sections are quite adequate. For the perturbed solitary wave discussed in this section, alternative perturbative methods, like that of Grimshaw,[11] might be more physical and easier than trying to work through the residual equations.

Wahlquist[12] and Kuznetsov and Mikhailov[13] report solutions obtained via Backlund transformations and the inverse scattering transform. Zagrodzinski and Jaworski[14] apply ideas similar to Shirafuji's to obtain what they dub "mixed" solutions, i.e., solitons perturbed by sine waves, for the sine-Gordon equation for general N.

VII. ACCURACY OF THE PERTURBATION SERIES

In Ref. 1, it is shown that the complementary perturbation series, one which gives the first few terms of the Fourier series of the theta function and the other which gives the Gaussian series, were very accurate for the ordinary cnoidal wave provided that each series was used in the proper regime (small wave amplitude for the Fourier series and large amplitude for the Gaussian series). In the worst case, i.e., that intermediate wave amplitude for which both series converge equally well or poorly, both gave the phase speed to within a relative error of 4.7% to zeroth order, and to within 0.027% to first order, where "zeroth" order refers to the phase speed of a linear sine wave in the Fourier case and a solitary wave on an infinite spatial interval in the Gaussian case.

For the double cnoidal wave, the overlap between the two complementary perturbation series is not quite so dramatic, but it is still good. Figures 1 and 2 compare regions in which the zeroth-order and first-order perturbation series give errors which are less than 10%. The error criterion is to take the largest of the three errors for c_1, c_2, and either T_{12} or R_{12} as appropriate using the modified relative error criterion

$$\text{Error} = (c_1^{\text{pert}} - c_1^{\text{exact}})/c, \tag{7.1}$$

where

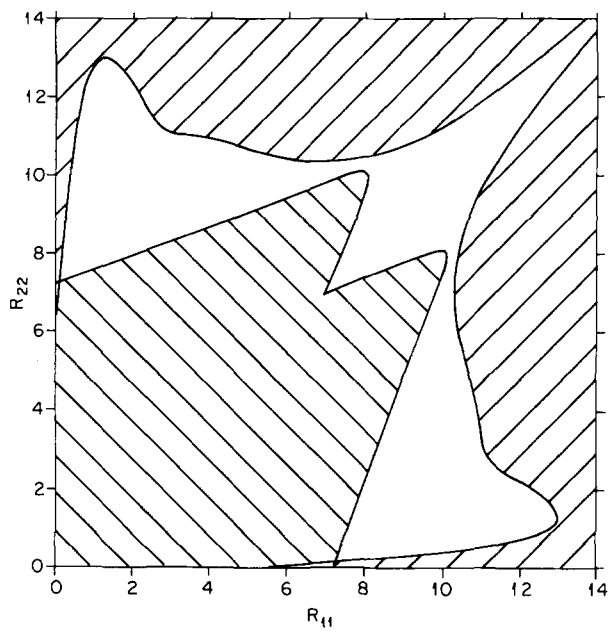

FIG. 1. The lines slanting from top right to bottom left denote that region in the $R_{11} - R_{22}$ plane where the error in all three of the quantities c_1, c_2 and R_{12}, which suffice to determine the theta function and the corresponding solution of the Korteweg–de Vries equation, is less than 10% for zeroth-order Gaussian perturbation theory, which is the double solitary wave approximation. The modified relative error is defined by Eqs. (7.1) and (7.2). The lines slanting from top left to bottom right are the 10% error region for the zeroth-order Fourier perturbation theory, which is equivalent to approximating the double cnoidal wave as the sum of two linear sine waves. The blank area is "no-man's land" where neither approximation is accurate within 10%.

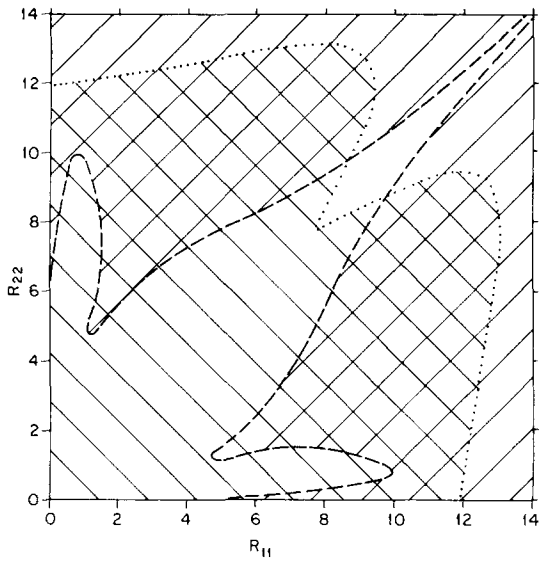

FIG. 2. Same as Fig. 1 except for the first-order Fourier and Gaussian approximations, which incorporate the first correction to the double solitary wave and double sine wave. The first-order theories overlap very well.

$$c = \text{larger of} \begin{cases} c_1 \\ c_1^{\text{linear sine wave}} \end{cases} = -39.4, \tag{7.2}$$

and similarly for c_2 and the off-diagonal theta matrix element. The reason for the modification, i.e., the replacement of the exact variable by its value in the linear limit, is that both phase speeds vanish along certain curves in the two-dimensional parameter space spanned by R_{11} and R_{22}, which implies infinite unmodified relative errors in the neighborhood of these curves even though the absolute errors may be very small.

Figures 1 and 2 show the principal branch of the double cnoidal wave with $k_1 = k_2 = 1$. Because the wavenumbers are identical, the graph is symmetric about the diagonal $R_{11} = R_{22}$. The neighborhood of this diagonal corresponds to a perturbed ordinary cnoidal wave of unit period. As explained in the preceding section, neither perturbation series can be expected to work well in these neighborhoods because both that derived in Sec. IV and the Gaussian series of Sec. V implicitly assume that the amplitudes of both waves are either very small or very large. However, the graphs show that the near-diagonal and near-axis regions where the Gaussian and Fourier perturbation series fail are quite narrow—almost invisible on the scale of the graph. This is a strong pragmatic justification for omitting a detailed treatment of the mixed Gaussian–Fourier perturbation series which, as noted in Sec. VI, can be calculated, but which would hardly ever be of any practical value.

Even outside these narrow perturbed-single-soliton areas, the zeroth-order perturbation curves do not quite overlap; there is a small region of moderate R_{11} and R_{22} where neither approximation gives all three dependent variables to within 10%. However including the first-order corrections to the sum of the two noninteracting linear sine waves and to the double solitary wave reduces the error to less than 10% everywhere except very close to the diagonals and the axes.

The physical implication is clear: The double cnoidal wave of the Korteweg–de Vries equation can always be considered both qualitatively and quantitatively to be either (i) the sum of two noninteracting sine waves; (ii) a pair of solitary waves of different heights, repeated with unit period over all x; or (iii) a single soliton plus a weak sinusoidal perturbation. When one wants to obtain numerical values for the double cnoidal wave, the perturbation series derived earlier will usually be adequate. If high accuracy is needed, it is straightforward to solve the residual equations numerically using the peturbation series to initialize the iteration.

The one serious complication is that the Fourier and Gaussian perturbation series involve different parameters—the Fourier expansion uses T_{11} and T_{22} while Gaussian employs R_{11} and R_{22}—and it is not possible to transform from one pair of parameters to the other unless one knows either T_{12} and R_{12}. In practical terms, this means that if one wants to make a contour plot of the phase speed c_1 as a function of T_{11} and T_{22} including such small values of these diagonal theta matrix elements that one passes into the double-soliton regime, one must use an iteration instead of a direct evaluation. One must guess T_{12} (in the large amplitude, double-soliton regime, one cannot calculate it from the Fourier perturbation series), perform a modular transformation as in Ref. 3 to obtain the three inverse theta matrix elements, apply the Gaussian perturbation series, determine the difference between the R_{12} obtained by the modular transformation and that calculated by the Gaussian perturbation series, transform back to T_{11}-T_{22} space, and guess a new value for T_{12} and so on. The fact that the off-diagonal theta matrix elements are unknowns rather than independent parameters is a considerable practical difficulty.

Fortunately, it is one that arises only when one is attempting to simultaneously explore the dynamics of double cnoidal waves in both the large and small amplitude regimes. If one is content instead to examine the double cnoidal wave strictly as the sum of two solitary waves, then one can stick to the inverse theta matrix elements R_{11} and R_{22} as parameters and use the Gaussian perturbation series alone. If one wants to investigate polycnoidal waves as a sum of quasilinear waves, the Fourier perturbation series is more than adequate.

VIII. SUMMARY

Following the plan outlined in Ref. 1, the problem of the double cnoidal wave for the Korteweg–de Vries equation has been reduced to four algebraic equations in four unknowns. Because the four functions of this set are defined only via infinite series, it is extremely advantageous to express these four residual functions in two quite different ways: one obtained by using the ordinary Fourier series of the theta function and then applying the theorems of Ref. 1, and a second representation derived via the alternative Gaussian series. These representations are mutually complementary in the sense that the Fourier representation, obtained independently by Nakamura,[4] is very efficient for small amplitude double cnoidal waves while the Gaussian representation, obtained here for the first time, is highly effective for large amplitude, i.e., when the double cnoidal wave is approximately equal to two solitary waves of unequal heights repeated periodically over all space.

It is also straightforward to solve the residual equations using perturbation theory. Comparisons with numerical solutions show that even the zeroth-order perturbation series have good overlap while the two first-order series cover almost all of parameter space with errors of 10% or less. By using the algebraic manipulation language REDUCE 2, it is trivial to extend the series to fairly high order for the principal branch of the double cnoidal wave (fourth order for the Fourier case and second order for the Gaussian series) so as to cover all the physically interesting regimes in parameter space.

The methods employed here, which explicitly use the properties of the Riemann theta function, are only applicable to partial differential equations which are exactly integrable by the periodic analog of the inverse scattering method, which is known as the "Hill's spectrum" procedure. Within this class, however, the ideas developed here extend very readily to other equations. For the Boussinesq water wave equation, for example, the calculations presented here can be repeated merely by altering the residual equations (and the appropriate line in the REDUCE 2 computer program) to use a new function $\zeta(m,n)$, where $\zeta(m,n)$ is defined (for the Korteweg–de Vries equation) by (2.11).

The Gaussian perturbation series is remarkable in that it converges most rapidly when the wave amplitude is large rather than small, which makes it well suited for exploring the effects of spatial periodicity on solitary waves. The Fourier perturbation series is useful, too, because its form is simpler and easier to evaluate than the Gaussian series and it remains accurate even for moderately large waves. Both series share the common property that it is not necessary to write down separate series for each of an infinite number of Fourier coefficients or the like: one need only have series for three parameters, and these determine the whole infinite series for the theta function, and thus for the double cnoidal wave itself.

Future work to calculate perturbation series for other partial differential equations integrable via the "Hill's spectrum" method is now in progress. It is hoped that the results will be useful whenever equations of soliton type are applied with spatially periodic boundary conditions, or wherever there is a high density of solitons so that soliton–soliton overlap is important.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation under grants OCE8108530 and OCE8305648.

APPENDIX A: PERTURBATION THEORY IN AN UNPHYSICAL REPRESENTATION

The companion paper (Ref. 3) has shown that via the "special" modular transformation, a given theta function can be expressed in a denumerably infinite number of ways. Each of these allowed representations involves theta functions of two "angle" variables, $X = k_1(x - c_1 t)$ and $Y = k_2(x - c_2 t)$, but in general the phase speeds c_1 and c_2 have no actual physical interpretation unless the representation is that unique one defined to be the "physical" representation in Ref. 3. Fortunately, the perturbation series given earlier automatically calculate in this "physical" representation so that c_1 and c_2 are the actual speeds at which individual peaks of the polycnoidal wave are moving.

Nonetheless, it is still of interest to see how perturbation theory can cope with the problem of calculating in an "unphysical" representation because this both provides an additional demonstration of the existence of an infinite number of alternative representations of the theta function and also illuminates the assumptions and details of the perturbation method. For simplicity, attention will be limited to the lowest-order Fourier case for a polycnoidal wave consisting of a sine wave of unit period and its second harmonic (plus very small high harmonics created by their interaction which will not be explicitly calculated).

Assuming that

$$T_{11},\ T_{22} \gg 1 \tag{A1}$$

the four residual equations are, to lowest order with common factors omitted,

$$\rho_{00} = \zeta(0,0) \tag{A2}$$

$$\rho_{10} = \zeta(1,0), \tag{A3}$$

$$\rho_{01} = \zeta(0,1) + e^{-2T_{11}-2T_{12}}\zeta(2,1), \tag{A4}$$

$$\rho_{11} = e^{-2T_{12}}\zeta(1,1) + \zeta(1,-1), \tag{A5}$$

where the zeta function for the Korteweg–de Vries equation is defined by

$$\zeta(m,n) \equiv 16\pi^4(k_1 m + k_2 n)^4 + 4\pi^2(k_1 m + k_2 n)(k_1 c_1 m + k_2 c_2 n) - 2A. \tag{A6}$$

[The zeta function satisfies the general symmetry relation $\zeta(m,n) = \zeta(-m,-n)$ as evident in (A6), and this has been used to simplify (A3) through (A5).]

In the physical representation for which $k_1 = 1$ and $k_2 = 2$, (A2) and (A3) may be solved to give

$$c_1 = -4\pi^2 + O(e^{-2T_{11}}, e^{-2T_{22}}), \tag{A7}$$

$$A = 0 + O(e^{-2T_{11}}, e^{-2T_{22}}), \tag{A8}$$

If one assumes

$$|T_{12}| \ll T_{11}, T_{22} \tag{A9}$$

as done implicitly in earlier sections, then the second term in ρ_{01} must be neglected to give

$$c_2 = -16\pi^2 + O(e^{-T_{11}}, e^{-2T_{22}}). \tag{A10}$$

Equation (A9) is the key assumption that ensures that we calculate in the physical representation. The phase speed c_2 is indeed that of a second harmonic of the linearized Korteweg–de Vries equation. The residual $\rho_{11} = 0$ gives

$$T_{12} = \log(3) = 1.0986. \tag{A11}$$

It is, however, equally possible to calculate in the unphysical representation $k_1 = k_2 = 1$. As stressed in the author's companion paper on the modular transformation,[3] the linear dispersion relation gives a unique phase speed for each wavenumber, so it is quite absurd to suppose that the two waves of different phase speeds which are the dominant terms in the Fourier series of a small amplitude double cnoidal wave can both have identical wavenumbers. (If wave-

numbers and phase speeds are the same, then the two waves are identical and we have an ordinary cnoidal wave which depends on but a single "angle" variable.) Nonetheless, it is still possible to represent the solution using a theta function with the unphysical wavenumber $k_2 = 1$ if (A9) is replaced by

$$T_{12} = -T_{11} + \Delta. \tag{A12}$$

The first two residuals are unaffected (to lowest order!) by the change in k_2 and by (A12), so the phase speed c_1 and constant of integration are still given by (A7) and (A8). The invariance of c_1 is in fact true to all orders in perturbation theory because a modular transformation that alters k_2 and Y does not affect X and c_1 at all as may be seen in Table I of Ref. 3. The invariance of A is also exact because the special modular transformation leaves the theta function unchanged, which means that after the angle variables have been converted to x and t, the theta function has the same dependence on space and time as before. The theta function must therefore satisfy the Hirota–Korteweg–de Vries equation with the same constant of integration A.

The other two residual equations, however, are quite drastically changed. When the wavenumbers are identical and $A = 0$,

$$\zeta(1,1) = 0 \tag{A13}$$

so that

$$\rho_{11} = e^{-2T_{12}}\zeta(1,1). \tag{A14}$$

The only way that $\rho_{11} = 0$ is if either (i) $T_{12} = \infty$, which is impossible since the theta series would diverge or (ii)

$$\zeta(1,1) = 0 \tag{A15}$$

which demands

$$c_2 = -28\pi^2. \tag{A16}$$

This is not the phase of any linear wave of the Korteweg–de Vries equation with an integer wavenumber.

Because of the large magnitude ot T_{12}, it is no longer legitimate to neglect the second term in ρ_{01}, which becomes [using (A12)]

$$\rho_{01} = \zeta(0,1) + e^{-2\Delta}\zeta(2,1), \tag{A17}$$

which gives

$$T_{12} = -T_{11} + 1.0986. \tag{A18}$$

These alterations in c_2 and T_{12} [from the values given in (A10) and (A11)] are exactly as listed in Table I of the companion paper by Boyd for a transformation by the modular generator $\mathbf{A}_2^{-1}$. Equation (A16) is the limit of the numerically calculated values of c_2 as given in Table II of the same paper, while (A10) gives the limit of what is called c_2^{mod} in the same table. Thus, there is a gratifying consistency between the numerical solutions of the residual equation, the perturbation theory, and the special modular transformation.

The lowest three terms of the theta function itself can be written in either representation,

$$\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix} = 1 + e^{-T_{11}}\cos(2\pi X) + e^{-T_{22}}\cos(2\pi Y) + e^{-T_{11}-T_{22}-2T_{12}}\cos(2\pi[X+Y]). \tag{A19}$$

In the "physical" representation [1,2], i.e., $k_1 = 1$ but $k_2 = 2$, the first two cosine terms are dominant in the limit of $T_{11}, T_{22} \gg 1$. In the "unphysical" representation [1,1], i.e., $k_1 = k_2 = 1$, (A18) implies

$$e^{-T_{11}-T_{22}-2T_{12}} = e^{-T_{22}}e^{T_{11}-2.2972} \gg e^{-T_{22}} \tag{A20}$$

for large T_{11}, so that the $\cos(2\pi Y)$ term is exponentially small in comparison to the "mixed" terms $\cos(2\pi[X+Y])$. This is as it should be because $\cos(2\pi[X+Y])$ is of wavenumber 2 in x and is in fact identical with the term which is written $\cos(2\pi Y)$ in the other representation.

APPENDIX B: THE RELATIONSHIP BETWEEN THE "TETRA-GAUSSIAN" DOUBLE SOLITON AND HIROTA'S DOUBLE SOLITON

As noted in the main body of this paper and the author's previous work,[1] the sum of the four Gaussians with peaks at the corners of the unit square, named the "tetra-Gaussian" and labeled by an upper case Greek Θ, can be given two interpretations. First, it is the lowest-order approximation to the full theta function series $\theta(X,Y)$. Second, it is an exact solution of the Hirota–Korteweg–de Vries equation for the spatially unbounded problem, representing two solitary waves of unequal height. This second interpretation is important because it justifies interpreting the double cnoidal wave as a double soliton when the wave amplitudes are large enough so that the tetra-Gaussian is an accurate approximation.

It therefore, is useful to explain how the tetra-Gaussian, which seemingly is very different, is physically equivalent to Hirota's own solution to the HKdV equation, which is

$$H(x,t) = 1 + e^{-\bar{\delta}_1 x + \bar{\delta}_1^3 t - \phi_1} + e^{-\bar{\delta}_2 x + \bar{\delta}_2^3 t - \phi_2} + \left(\frac{\bar{\delta}_1 - \bar{\delta}_2}{\bar{\delta}_1 + \delta_2}\right)^2 \times \exp(-(\bar{\delta}_1 + \bar{\delta}_2)x + (\bar{\delta}_1^3 + \bar{\delta}_2^3)t - \phi_1 - \phi_2). \tag{B1}$$

The tetra-Gaussian in contrast is

$$\Theta(x,t) = \sum_{n_1 = \pm 1/2}\sum_{n_2 = \pm 1/2} \exp(-\{(R_{11}/2)(X+n_1)^2 + R_{12}(X+n_1)(Y+n_2) + (R_{22}/2)(Y+n_2)^2\}) \tag{B2}$$

or written in terms of x and t

$$\Theta(x,t) = \exp(-(\alpha/2)x^2 - \beta xt - (\gamma/2)t^2 - (R_{11}/8) - (R_{22}/8)) \times \sum_{n_1 = \pm 1/2}\sum_{n_2 = \pm 1/2} \exp(-\{(\delta_1 n_1 + \delta_2 n_2 + \delta_p)x + (\epsilon_1 n_1 + \epsilon_2 n_2 + \epsilon_p)t\}) \times \exp(-\{R_{12}n_1 n_2 + \Phi_1 n_1 + \Phi_2 n_2 + \Phi_p\}) \tag{B3}$$

where the Greek letters are related to the theta matrix elements and k_1, k_2, etc., via (2.8) through (2.19). Thus, Hirota's solution is an unsymmetrical sum of four exponentials of linear arguments and is spatially unbounded, whereas the tetra-Gaussian is a symmetrical sum of four exponentials of

quadratic arguments. Because of (i) the form of the function $\zeta(i,j)$ which appears in the residual equation (2.22), (2.23), and (2.26); and (ii) the second logarithmic derivative transformation, these differences are almost entirely cosmetic if one matches the pseudowavenumbers, i.e.,

$$\bar{\delta}_1 = \delta_1, \quad \bar{\delta}_2 = \delta_2. \tag{B4}$$

It was stressed in the author's previous work[1] that the reason one can prove that all but four of the residual equations $\rho_{jk} = 0$ are redundant is because $\zeta(i,j)$ depends only on differences in the exponentials of a pair of terms in the theta function whose interaction in the bilinear HKdV equation is described by $\zeta(i,j)$. This implies that if $H(x,t)$ is a solution of the HKdV equation, then $\exp[\nu x + \omega t + \Xi]H(x,t)$ is also a solution for arbitrary constants ν, ω, and Ξ. This theorem was widely used by Hirota himself a decade ago to manipulate his solutions into convenient form. Here, recalling that the explicit, exact solution of the residual equations for the tetra-Gaussian (which is also the lowest-order approximate solution for the full θ-series) implies that $\epsilon_1 = \delta_1{}^3 - 12\alpha\delta_1$, $\epsilon_2 = \delta_2{}^3 - 12\alpha\delta_2$, and $\exp[-R_{12}] = (\delta_1 - \delta_2)^2/(\delta_1 + \delta_2)^2$, one can verify through routine multiplication that $\exp[\nu x + \omega t + \Xi]H(x,t)$ matches $\Theta(x,t)$ except for the dependence of the latter on α, β, and γ provided that

$$\nu = \tfrac{1}{2}(\delta_1 + \delta_2), \tag{B5}$$

$$\omega = \tfrac{1}{2}(\delta_1{}^3 + \delta_2{}^3), \tag{B6}$$

$$\Xi = -R_{11}/8 - R_{22}/8 + \Phi_p - \phi_1/2 - \phi_2/2 - R_{12}/4, \tag{B7}$$

and that one adjusts the phase factors ϕ_1 and ϕ_2 in the angle variables X and Y, which determine Φ_1 and Φ_2 in (B2) via $\Phi_1 = R_{11}\phi_1 + R_{12}\phi_2$ and $\Phi_2 = R_{12}\phi_1 + R_{22}\phi_2$, so that

$$\Phi_1 = \phi_1 + R_{12}/2, \tag{B8}$$

$$\Phi_2 = \phi_2 + R_{12}/2. \tag{B9}$$

The two phase factors in X and Y are neither more nor less than what is needed to match the two phase factors in $H(x,t)$ and vice versa.

Since $\zeta(i,j)$ is independent of γ, it follows that $\exp[-(\gamma/2)t^2]H(x,t)$ is a solution if $H(x,t)$ is. The function $\zeta(i,j)$ does depend on β, but only in the combination of $\beta - A$. Thus, if $H(x,t)$ solves the HKdV equation with $A = 0$, then $\exp[-\beta x t]H(x,t)$ is a solution of the HKdV equation with the new constant of integration $A = \beta$. This same reasoning explains why Fourier series numerical integration of the HKdV equation instead of the KdV equation, which is otherwise tempting because the Fourier series of the theta function converges much more rapidly than that for the mermorphic function which is the corresponding solution of the KdV equation, will not work unless A is known in advance: There is only a single value of A which the HKdV equation has a periodic solution. Arbitrary choices of A will yield solutions that are the products of a periodic function with $\exp[-(\text{const})xt]$. This is strictly a numerical difficulty, however; neither β nor A has any effect on the solution of the Korteweg–de Vries equation because the $\exp[-\beta x t]$ factor is automatically eliminated when the second logarithmic derivative is taken.

The factor of $\exp[-(\alpha/2)x^2]$ does alter $u(x,t)$, but only by the addition of a constant and simultaneously a shift in all the phase speeds by the same constant. Stated formally, one can easily show from the form of $\zeta(i,j)$ (or from the theorem given in Sec. VII of the author's previous work) that if $H(x,t)$ is a solution of the HKdV equation with $u(x,t) = 12(\ln H)_{xx}$ as the corresponding KdV solution, then $\exp[-(\alpha/2)x^2]H(x + 12\alpha t, t)$ is also an HKdV solution with the new constant of integration $A' = A - 6\alpha^2$ with

$$v(x,t) = -12\alpha + u(x + 12\alpha t, t) \tag{B10}$$

as the corresponding solution of the Korteweg–de Vries equation. Thus, aside from the α dependence in (B10), the tetra-Gaussian is physically equivalent to Hirota's double-soliton HKdV solution, even though their mathematical form is rather different.

APPENDIX C: THE "TETRA-GAUSSIAN" AND THE GEOMETRY OF THE X-Y PLANE

For large R_{11}, R_{22}, one can accurately approximate the full theta function series by a tetra-Gaussian and deduce a number of simple facts that have been exploited here and in Ref. 2. First, note that, using Θ to denote the tetra-Gaussian as in Appendix B,

$$\ln\Theta \equiv \ln\Bigg[\sum_{n_1=-1/2}^{1/2}\sum_{n_2=-1/2}^{1/2}\exp\Bigg(-\Bigg\{\Big(\frac{R_{11}}{2}\Big)(X+n_1)^2 + R_{12}(X+n_1)(Y+n_2) + \Big(\frac{R_{22}}{2}\Big)(Y+n_2)^2\Bigg\}\Bigg)\Bigg], \tag{C1}$$

which by extracting the common factor is

$$= -(R_{11}/2)X^2 + R_{12}XY + (R_{22}/2)Y^2 + \ln\Bigg[\sum_{n_1=-1/2}^{1/2}\sum_{n=-1/2}^{1/2}\exp(-R_{11}Xn_1 - R_{22}Yn_2 - R_{12}Xn_2 - R_{12}Yn_1)\Bigg]. \tag{C2}$$

When we take the second derivative of $\ln\Theta$, the quadratic terms in X^2, XY, and Y^2 are converted to a constant (-12α), so the shape of the double soliton is determined entirely by the remaining logarithm in (C2), i.e.,

$$L \equiv \ln\Bigg[\sum_{n_1=-1/2}^{1/2}\sum_{n_2=-1/2}^{1/2}\exp(-R_{11}Xn_1 - R_{22}Yn_2 - R_{12}Xn_2 - R_{12}Yn_1)\Bigg]. \tag{C3}$$

As done in Appendix B, one can then show that the sum of the four exponentials with linear arguments in (C2) is equivalent to Hirota's sum of four linear exponentials that generate the double solitary wave in the spatially unbounded problem.

Here, a different strategy will be adopted. When R_{11} and R_{22} are very large, the "tetra-Gaussian" has four narrow peaks at each of four corners of the unit square $X = \pm\frac{1}{2}$, $Y = \pm\frac{1}{2}$. Over most of the square, Θ is dominated by a single term. The logarithm of a single exponential of linear argument in (C2) can be evaluated explicitly to give a result linear in X and Y, which is then eliminated by taking two derivatives. Thus, solitons occur only where at least two peaks of the tetra-Gaussian are of comparable magnitude.

One such region is the neighborhood of the positive Y axis where the important peaks are $n_1 = \pm\frac{1}{2}$, $n_2 = -\frac{1}{2}$ and

$$L \doteq \ln[2\cosh(R_{11}X/2 + R_{12}Y/2 - R_{12}/4)] + R_{22}Y/2 + R_{12}X/2. \quad \text{(C4)}$$

The valley in the graph of Θ [which corresponds to a ridge of the function $U(X,Y)$ graphed in Figs. 7, 8, and 10 of Ref. 2] occurs along the line where the argument of the hyperbolic cosine is 0, i.e.,

$$R_{12}Y = -R_{11}X + R_{12}/2. \quad \text{(C5)}$$

Repeating the argument along the negative Y axis gives (C5) again except for a sign change for the Y-intercept, $R_{12}/2$. Thus, one finds, as quoted in Sec. VI of Ref. 2, that the slopes of the soliton valleys are $(-R_{11}/R_{12})$ and by similar reasoning, $(-R_{12}/R_{22})$.

Using the definitions $\delta_1 = R_{11}k_1 + R_{12}k_2$, $X \equiv k_1(x - c_1 t)$, etc., as in (5.7) and (2.4) above, one can write

$$L = \ln(\cosh[(\delta_1/2)X + (\epsilon_1/2)t - R_{12}/4]) + [*], \quad \text{(C6)}$$

where the $[*]$ denotes terms that will be eliminated by differentiation. Then

$$u(x,t) \equiv 12\frac{d^2}{dx^2}L = 3{\delta_1}^2\,\mathrm{sech}^2[(\delta_1/2)\{x + (\epsilon_1/\delta_1)t - R_{12}/(2\delta_1)\}]. \quad \text{(C7)}$$

Thus, the soliton whose width and amplitude are determined by the diagonal inverse theta matrix element R_{11} corresponds to a trough in the graph of $\theta(X,Y)$ which runs roughly parallel to the Y axis. Repeating the analysis for negative Y gives (C7) again except for a change of sign in R_{12}. Now, the region around the origin is where the two soliton troughs turn and merge. The jump represented by the sign change in R_{12} is therefore the collisional phase shift, which is then

$$\text{phase shift} = R_{12}/\delta_1. \quad \text{(C8)}$$

The tilting of the soliton troughs so that they only approximately parallel the X and Y axes is intimately related to this collisional phase shift. Since the full theta series is dominated within the unit square entirely by the four peaks of the tetra-Gaussian, it follows that the soliton valleys must intercept the edges of the unit square at the same value of $X(Y)$ for the trough paralleling the $Y(X)$ axis, to within $O(\exp[-R_{11}/2], \exp[-R_{22}/2])$, or the theta function will not be periodic. Were it not for the phase shift, the troughs could preserve periodicity simply by running parallel to the axes. As it is, the tilt insures that the troughs, whose equations are

$$R_{12}Y = -R_{11}X \pm R_{12}/2, \quad (+)Y > 0, \ (-)Y < 0, \quad \text{(C9)}$$

both intersect the edges of the unit square, $Y = \pm\frac{1}{2}$, at $X = 0$. As explained in Sec. VI of Ref. 2, this tilting of trough lines also implies that the phase velocities are not the speeds of the "free" solitary waves, i.e., the rate at which the solitons travel when not enmeshed in a collision; c_1 and c_2 are rather the time-averaged velocities of the peaks of $u(x,t)$.

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The special modular transformation for polycnoidal waves of the Korteweg–de Vries equation

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(Received 22 March 1984; accepted for publication 22 June 1984)

The modular transformation of the Riemann theta function is used to show that the implicit dispersion relation for the N-polycnoidal waves of the Korteweg–de Vries equation has a countable infinity of branches for $N \geqslant 2$. Although the transformation also implies that each branch or mode can be written in a countable infinity of ways, it is also shown that there is a unique "physical" representation for each mode such that the parameters of the theta function can be interpreted as wavenumbers and amplitudes in the limit of either very small or very large amplitude. Unfortunately, the small amplitude "physical" representation is different (by a modular transformation) from the large amplitude "physical" representation for a given mode, but this difference explains an apparent paradox as described in the text. The general modular transformation expresses the theta function in terms of complex wavenumbers, phase speeds, and coordinates that have no physical relevance to the Korteweg–de Vries equation, but it is shown that for $N \geqslant 2$, there is a subgroup, here dubbed the "special modular transformation," which gives a real result. This subgroup is explicitly constructed for general N and presented as a table for $N = 2$.

PACS numbers: 02.30.Jr, 02.60.Lj, 02.30.Qy

I. INTRODUCTION

This present work will focus on four themes. The first is the specialization of the general modular transformation of the theta function to that subgroup, here dubbed the "special" modular transformation, which is relevant to the Korteweg–de Vries equation. This construction is done in Secs. II, III, and IV, beginning with a description of the general transformation, then explicitly constructing the "special" transformation for general N, and finally discussing in detail the special case $N = 2$, which is the subject of the companion papers by the author.[1]

The second half of the paper will discuss in turn the three remaining issues: the multiplicity of roots of the N-polycnoidal wave dispersion relation for $N \geqslant 2$ (Sec. V); the so-called "paradox of the wavenumbers" (Sec. VI); and finally which of the infinite number of mathematically equivalent ways of writing the theta function is the "physical" representation in which the wavenumbers and phase speeds are those of the actual solitons or sine waves of the solution (Sec. VII). Before turning to the transformation itself, it is useful to describe each of these last three themes in enough detail to motivate the technical discussion of Secs. II, III, and IV.

The implicit dispersion relation for N-polycnoidal waves, derived in Refs. 1 and 2, is linear in all the unknowns for the special case $N = 1$ (the ordinary cnoidal wave discovered by Korteweg and de Vries in 1895) and thus has a unique solution. However, for $N \geqslant 2$, the dispersion relation is transcendentally nonlinear—that is, the algebraic equations we must solve are defined by infinite series in one or more unknowns—so an infinite number of roots is at least possible. The mere existence of the modular transformation raises this to a near certainty. As reviewed in Ref. 1, the N-polycnoidal wave is the second logarithmic derivative with respect to x of the N-dimensional Riemann theta function $\theta \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}(\mathbf{T}, \boldsymbol{\zeta})$ whose N arguments are the "phase variables"

$$\zeta_j \equiv k_j(x - c_j t) + \phi_j, \tag{1.1}$$

where x is the spatial coordinate, t is time, and where the constants k_j, c_j and ϕ_j are the jth wavenumber, phase speed, and phase factor, respectively. The coefficients of the N-dimensional Fourier series in the ζ_j of the theta function are completely determined by the elements of the symmetric $N \times N$ "theta matrix" $\mathbf{T}$ as shown explicitly in Eq. (2.1) below. The special modular transformation allows the ζ_j and t_{ij} (theta matrix elements) to be simultaneously altered in a countable infinity of ways without changing the sum of the infinite series. Thus, a single root of the dispersion relation generates the solution at an infinite number of discrete points in parameter space.

A more precise picture can be obtained by looking at the limits of either very large amplitude or very small amplitude where the phase speeds c_j are known analytically,[1] and examining what we shall name the "modes" of the wave. In the small amplitude regime, the diagonal theta matrix elements $t_{ii} \gg 1$ and the N-polycnoidal wave can be approximated as the sum of N sine waves each proportional to $\cos(2\pi\zeta_j)$ for a different j. Without loss of generality,[2] one can always rescale the N-polycnoidal wave to unit period. For $N = 2$, we can thus always take $k_1 = 1$, but strict periodicity in x is preserved if $k_2 = n$, where n is any integer $\geqslant 2$. Because each different choice for k_2 gives a distinct solution, one whose graph is distinct from that for any other choice of n, we will refer to the different possibilities as "modes" and write their wavenumbers in square brackets separated by a comma, viz., $[1,n]$.

Now when the modular transformation is applied to a theta function, it alters a wavenumber by an integer. Thus, each mode $[1,n]$ can always be expressed in terms of a theta

 0022-2488/84/123415-09$02.50

function with $k_1 = 1$ and $k_2 = 2$. Thus, the dispersion relation for the gravest [1,2] mode has roots corresponding to the modular transformations of all the other modes [1,n]. In Sec. V, we will tighten this argument and look at the multiple roots of the dispersion relation in some detail.

The "paradox of wavenumbers" arises because one can equally well define the "modes" of the N-polycnoidal wave in terms of the limit of large amplitude. In this regime, the peaks of the wave are very tall and narrow and essentially indistinguishable (because of their narrowness) from the solitary waves (solitons) of the spatially unbounded (as opposed to periodic) Korteweg–de Vries equation. There are solitons of N different sizes on each interval and, as explained in Ref. 1, the role of the wavenumbers k_j is quite different from that in the small amplitude limit in that the k_j specify how many solitons of the jth size appear on each spatial period. To emphasize the different role of wavenumbers, we shall denote the modes as identified in the near-soliton regime by writing the wavenumbers in braces.

The "paradox" referred to above is that $\{1,1\}$ is now the gravest $N = 2$ mode (one tall soliton and one short soliton on each unit spatial interval), whereas the simplest small amplitude mode is [1,2]. Since the linear dispersion relation gives a unique phase speed in the limit of infinitesimal waves, it is not possible to superimpose two sine waves with $k_1 = k_2 = 1$ and obtain two distinct phase speeds; such a mode would collapse into an ordinary ($N = 1$) cnoidal wave. Since the wavenumbers are fixed parameters of the implicit dispersion relation, this apparent contradiction about the identity of the gravest mode is very confusing.

In Sec. VI, this paradox will be resolved with the aid of the special modular transformation. There, it is shown that if one sets $k_1 = k_2 = 1$ and begins to vary the amplitude downwards in small steps, solving the dispersion relation numerically at each step starting from the known soliton velocities, one will eventually compute the [1,2] small amplitude mode. However, the numerical phase speeds obtained with $k_1 = k_2 = 1$ will not be those of the [1,2] mode directly, but rather the modular transformation of these phase speeds. Thus, the paradox is resolved: the gravest [1,2] and $\{1,1\}$ modes are indeed the same, continuous mode, but the equivalence can be demonstrated only via the special modular transformation.

This in turn raises the third issue. Given that a particular N-polycnoidal wave can be written in a countable infinity of ways thanks to the modular transformation, what representation, if any, is best? In the limit of very large or very small amplitude, we have already answered this question: For the gravest $N = 2$ mode, for example, the [1,2] ($\{1,1\}$) representation is best for small (large) amplitude because the phase speeds can then be physically interpreted as the actual phase speeds of the two linear sine waves or of the two solitons, respectively. What is to be done for intermediate amplitude, however? In Sec. VII, we will attempt to answer this question and give several alternative ways of quantifying the (thus far) vague meaning of "small amplitude" and "large amplitude."

The final section of the paper is a summary and prospectus.

II. THE GENERAL MODULAR TRANSFORMATION

The N-polycnoidal wave is the second logarithmic derivative with respect to x of the N-dimensional Riemann theta function $\theta\begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix}(\mathbf{T},\boldsymbol{\zeta})$, where the N arguments ("phase variables") are $\boldsymbol{\zeta} = (\zeta_1,\zeta_2,\ldots,\zeta_n)$ with $\zeta_j = k_j(x - c_j t) + \phi_j$ as in (1.1) above and where the theta function is defined by the uniformly convergent sum

$$\theta\begin{bmatrix}\boldsymbol{\epsilon}\\ \boldsymbol{\epsilon}'\end{bmatrix}(\mathbf{T},\boldsymbol{\zeta}) = \sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty}\cdots\sum_{n_N=-\infty}^{\infty}\exp\left[\pi i\left(\sum_{i=1}^{n}\sum_{j=1}^{n}t_{ij}\times\left(n_i+\frac{\epsilon_i}{2}\right)\left(n_j+\frac{\epsilon_j}{2}\right)+2\sum_{i=1}^{n}\left(n_i+\frac{\epsilon_i}{2}\right)\left(\zeta_i+\frac{\epsilon_i'}{2}\right)\right)\right], \tag{2.1}$$

where $\boldsymbol{\epsilon} = (\epsilon_1,\epsilon_2,\ldots,\epsilon_N)$ and $\boldsymbol{\epsilon}' = (\epsilon_1', \epsilon_2',\ldots,\epsilon_N')$ are together the "characteristic" of the theta function and the t_{ij} are the elements of the $N \times N$ symmetric "theta matrix" $\mathbf{T}$. In Ref. 1 and also the works of Nakamura,[3] Hirota and Ito,[4] and their collaborators, the details of calculating the phase speeds c_j and off-diagonal theta matrix elements ($t_{ij}, i \neq j$) ["unknowns"] in terms of the wavenumbers k_j and diagonal theta matrix elements t_{ii} ["parameters"] are explained. In this work, however, we shall concentrate solely on transformations of the theta function.

The most general transformations are lucidly described in a recent book by Rauch and Farkas.[5] So as to conform with their notation and that of most other mathematics texts, this paper will use theta matrix elements t_{ij} that are imaginary in contrast to the real matrix elements T_{ij} and R_{ij} which are more convenient in the two companion papers (Ref. 1). The results given in Table I, however, are notation-independent as explained in the table caption. If N is the dimensionality of the theta function (mathematicians often use g for N because N is also the "genus" of the Riemann surface associated with the theta function), then the transformations are generated by a $(2N)\times(2N)$ dimensional matrix $\mathbf{M}$ which is a member of Sp(N,Z), the so-called "homogeneous symplectic modular group." The term "symplectic" means that if one defines an $(2N)\times(2N)$ matrix $\mathbf{J}$ via

$$\mathbf{J} \equiv \begin{pmatrix}\mathbf{0}_N & -\mathbf{I}_N\\ -\mathbf{I}_N & \mathbf{0}_N\end{pmatrix},$$

where $\mathbf{0}_N$ is the $N \times N$ matrix whose elements are all zeros and $\mathbf{I}_N$ is the $N \times N$ identity matrix, then for any matrix $\mathbf{M}$ in the general $2N \times 2N$ symplectic group,

$$\mathbf{M}\mathbf{J}\mathbf{M}^T = \mathbf{J}, \tag{2.2}$$

where $\mathbf{M}^T$ is the transpose of $\mathbf{M}$. One can show that (2.2) implies

$$\det|\mathbf{M}| = \pm 1, \tag{2.3}$$

where "det" denotes the determinant. "Modular" denotes that subgroup of the general symplectic group whose matrix elements are all integers. Rauch and Farkas[5] explain why $\mathbf{M}$ must be both symplectic and modular, but their careful and readable exposition will not be repeated here.

The individual transformations are actually expressed in terms of submatrices of **M**, so Rauch and Farkas write **M** in the block form

$$\mathbf{M} \equiv \begin{pmatrix} \mathbf{D} & \mathbf{C} \\ \mathbf{B} & \mathbf{A} \end{pmatrix}, \tag{2.4}$$

where **A**, **B**, **C** are all $N \times N$ matrices. They prove the following.

Theorem: (Modular Transformation) If **M** is a member of the $(2N)\times(2N)$ homogeneous symplectic modular group and if **A**, **B**, **C**, and **D** are its $(N \times N)$ submatrices as defined by (2.4) above, then if

$$\hat{\boldsymbol{\xi}} = [(\mathbf{CT} + \mathbf{D})^T]^{-1}\boldsymbol{\xi}, \tag{2.5}$$

$$\hat{\mathbf{T}} = (\mathbf{AT} + \mathbf{B})\ (\mathbf{CT} + \mathbf{D})^{-1}, \tag{2.6}$$

where **T** is symmetric and positive definite imaginary and

$$\hat{\boldsymbol{\epsilon}} = \mathbf{D}\boldsymbol{\epsilon} - \mathbf{C}\boldsymbol{\epsilon}' + \text{diag}\,(\mathbf{CD}^T), \tag{2.7}$$

$$\hat{\boldsymbol{\epsilon}}' = -\mathbf{B}\boldsymbol{\epsilon} + \mathbf{A}\boldsymbol{\epsilon}' + \text{diag}\,(\mathbf{AB}^T), \tag{2.8}$$

where diag (**R**) is the vector-valued function of an arbitrary square matrix that returns the diagonal matrix elements of its argument as its result, i.e.,

$$\text{diag}\,(\mathbf{R}) \equiv \begin{pmatrix} r_{11} \\ r_{22} \\ \vdots \\ r_{NN} \end{pmatrix}, \tag{2.9}$$

then

$$\theta\begin{bmatrix} \hat{\boldsymbol{\epsilon}} \\ \hat{\boldsymbol{\epsilon}}' \end{bmatrix}(\hat{\boldsymbol{\xi}},\hat{\mathbf{T}}) = K \exp\left[\pi i\left(\sum_{k=1}^{N}\sum_{l=1}^{N} P_{kl}\xi_k\xi_l\right)\right]\theta\begin{bmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{\epsilon}' \end{bmatrix}(\boldsymbol{\xi},\mathbf{T}), \tag{2.10}$$

where the P_{kl} are the elements of the $N \times N$ matrix **P**, where

$$\mathbf{P} = (\mathbf{CT} + \mathbf{D})^{-1}\mathbf{C} \tag{2.11}$$

and where K is a constant dependent on **M**, $\boldsymbol{\epsilon}$, and $\boldsymbol{\epsilon}'$. Furthermore, $\hat{\mathbf{T}}$ is a theta matrix, i.e., symmetric and positive definite imaginary.

This theorem is far too general for the theory of the Korteweg–de Vries equation. First, the Korteweg–de Vries solution $u(x,t)$ is proportional to the second logarithmic derivative with respect to x of the theta function, so the constant K in (2.10), which is explicitly computed by Rauch and Farkas, is irrelevant to the theory of the Korteweg–de Vries equation and shall be ignored here.

Second, since the theta matrix **T** is positive definite imaginary, i.e., it must be complex, most of the transformations described by the theorem will yield complex phase variables $\hat{\xi}_j$ even if the untransformed variables are all real. Since complex coordinates are physically meaningless for the waves of the Korteweg–de Vries equation,[6] it follows that one loses nothing by concentrating only on that subgroup of transformations which yields real coordinates.

Inspecting (2.5) reveals two possibilities for such a subgroup: (i) $\mathbf{D} = 0$, in which case $\hat{\xi}$ is pure imaginary and all the factors of $i = \sqrt{-1}$ in (2.5) and the theta series (1.2) cancel to give a series involving real x and t only or (ii) $\mathbf{C} = 0$ so that $\hat{\xi}$ is real if ξ is real. The first possibility is equivalent to applying the Poisson summation method to rewrite the Fourier series of the theta function as a series of Gaussian functions as explained in an earlier paper by the author.[2] Strictly speaking, the Poisson sum is merely the special case $\mathbf{C} = -\mathbf{I}_N, \mathbf{B} = \mathbf{I}_N$. One can easily show, however, that using the most general **C**, **B** allowed by the symplectic condition (2.2) is equivalent to possibility (ii) for some **A**, **B** followed by Poisson summation. Consequently, (i) adds nothing to (ii) except the possibility of Poisson summation which was already thoroughly explored in earlier work. Therefore, the rest of this article will focus on the second case $\mathbf{C} = 0$. Keeping **T** pure imaginary then requires that $\mathbf{B} = 0$, so the general sympletic modular transformation has been reduced to those for which **A** and **D**, the diagonal submatrices, are the only nonzero blocks.

By substituting such a block diagonal **M** into the symplectic condition (2.2) and noting

$$\mathbf{M}^T = \begin{pmatrix} \mathbf{D}^T & \mathbf{0} \\ \mathbf{0} & \mathbf{A}^T \end{pmatrix} \tag{2.12}$$

one can show that the symplectic condition is satisfied if and only if

$$\mathbf{A} = [\mathbf{D}^{-1}]^T. \tag{2.13}$$

Rauch and Farkas[5] give a complete set of that finite number of generators whose products and inverse give the most general symplectic matrix which is also modular, i.e., has integral elements. For the special case considered here, one can discuss these $(2N)\times(2N)$ generating matrices in terms of a single $N \times N$ block (say the **A** block) because the rest of **M** is specified uniquely by $\mathbf{B} = \mathbf{0}$, $\mathbf{C} = \mathbf{0}$, and $\mathbf{D} = [\mathbf{A}^T]^{-1}$ according to (2.13). In the next section, these generators will be explicitly constructed.

III. THE SPECIAL MODULAR TRANSFORM

The modular transformation with $\mathbf{B} = \mathbf{C} = \mathbf{0}$ so the **M** is block diagonal will be referred to as the "special" modular transformation. As shown in the previous section, the "special" transformation is, excluding Poisson summation, the most general transformation of theta functions which is physically relevant to polycnoidal waves of the Korteweg–de Vries equation. It is useful to restate the theorems of the previous section for this special case.

Theorem: (special modular transformation) Let

$$\hat{\boldsymbol{\xi}} = \mathbf{A}\boldsymbol{\xi}, \tag{3.1}$$

$$\hat{\mathbf{T}} = \mathbf{ATA}^T, \tag{3.2}$$

$$\hat{\boldsymbol{\epsilon}} = [\mathbf{A}^{-1}]^T\boldsymbol{\epsilon}, \tag{3.3}$$

$$\hat{\boldsymbol{\epsilon}}' = \mathbf{A}\boldsymbol{\epsilon}', \tag{3.4}$$

where **A** is the lower right-hand block of a block-diagonal matrix **M** of the symplectic modular group. (The general form of **A** is constructed below.) Then

$$\theta\begin{bmatrix} \boldsymbol{\epsilon} \\ \hat{\boldsymbol{\epsilon}}' \end{bmatrix}(\hat{\boldsymbol{\xi}};\hat{\mathbf{T}}) = K\theta\begin{bmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{\epsilon}' \end{bmatrix}(\boldsymbol{\xi};\mathbf{T}), \tag{3.5}$$

where K is a constant.

Note that the Gaussian factor has disappeared because the matrix **P** of the general theorem is now identically zero; the special transformation takes a theta Fourier series directly into another theta Fourier series.

The generators are of two classes. For each, one begins with the $N \times N$ identity matrix and modifies it according to a prescription given by Rauch and Farkas. For the first class, ${}^{+}A_{ij}$ in their notation with i,j restricted so that $i \neq j$, add -1 to the (j,i) element of the identity matrix. For the second class D_i change the sign of the (i,i) element of the identity matrix. Rauch and Farkas also include the inverses of the ${}^{+}A_{ij}$ in their generator set as the ${}^{-}A_{ij}$; the D_i are their own inverses. (The ${}^{-}A_{ij}$ are obtained by adding $+1$ to the (j,i) element of the identity matrix.) One thus obtains a complete (but not necessarily minimal) generating set with $2N^2 - N$ members. The statement that this set is the complete generator of the special transformations means that the most general $N \times N$ matrix A which appears in (3.1)–(3.3) is the product of an arbitrary number of the generating matrices each raised to an arbitrary, non-negative power, i.e., if one adopts the revised notation of labeling the generators A_i, $i = 1,2,\ldots,2N^2 - N$, then the most general transformation is

$$A = A_{i_1}^{n_1} A_{i_2}^{n_2} A_{i_3}^{n_3} \cdots A_{i_m}^{n_m}, \tag{3.6}$$

where $n_j \geqslant 0$, $1 \leqslant i_j \leqslant 2N^2 - N$ but are otherwise arbitrary; m, the number of factors, is arbitrary also. The generators do not commute even for the special transformation, so (3.6) usually cannot be simplified.

TABLE I. The transformations produced by the generators of the special modular group $\mathbf{A}_1$ and $\mathbf{A}_2$, and their inverses for $N = 2$ (double cnoidal wave). The plus signs correspond to $\mathbf{A}_1$; the minus signs to $\mathbf{A}_1^{-1}$ and $\mathbf{A}_2^{-1}$. The ($\hat{}$) quantities are the new variables created by the transformation. The matrices whose elements are T_{ij} and R_{ij} are explained in Boyd[1]; the T_{ij} transform exactly as those of the usual imaginary theta matrix elements t_{ij} used by mathematicians. The k_i and c_i are the wavenumbers and phase speeds that appear in the "angle" variables X and Y when the special modular transformation is applied to the double cnoidal wave of the Korteweg–de Vries equation.

$\mathbf{A}_1$ (and $\mathbf{A}_1^{-1}$):

$$\begin{pmatrix}\hat{X}\\ \hat{Y}\end{pmatrix} = \begin{pmatrix}X \pm Y\\ Y\end{pmatrix},$$

$$\begin{pmatrix}\hat{T}_{11} & \hat{T}_{12}\\ \hat{T}_{12} & \hat{T}_{22}\end{pmatrix} = \begin{pmatrix}[T_{11} \pm 2T_{12} + T_{22}] & [T_{12} \pm T_{22}]\\ [T_{12} \pm T_{22}] & [T_{22}]\end{pmatrix},$$

$$\begin{pmatrix}\hat{R}_{11} & \hat{R}_{12}\\ \hat{R}_{12} & \hat{R}_{22}\end{pmatrix} = \begin{pmatrix}[R_{11}] & [R_{12} \mp R_{11}]\\ [R_{12} \mp R_{11}] & [R_{11} \mp 2R_{12} + R_{22}]\end{pmatrix},$$

$$\begin{pmatrix}\hat{k}_1\\ \hat{k}_2\end{pmatrix} = \begin{pmatrix}k_1 \pm k_2\\ k_2\end{pmatrix},$$

$$\begin{pmatrix}\hat{c}_1\\ \hat{c}_2\end{pmatrix} = \begin{pmatrix}[k_1c_1 \pm k_2c_2]/[k_1 \pm k_2]\\ k_2\end{pmatrix},$$

$\mathbf{A}_2$ (and $\mathbf{A}_2^{-1}$):

$$\begin{pmatrix}\hat{X}\\ \hat{Y}\end{pmatrix} = \begin{pmatrix}X\\ Y \pm X\end{pmatrix},$$

$$\begin{pmatrix}\hat{T}_{11} & \hat{T}_{12}\\ \hat{T}_{12} & \hat{T}_{22}\end{pmatrix} = \begin{pmatrix}[T_{11}] & [T_{12} \pm T_{11}]\\ [T_{12} \pm T_{11}] & [T_{11} \pm 2T_{12} + T_{22}]\end{pmatrix},$$

$$\begin{pmatrix}\hat{R}_{11} & \hat{R}_{12}\\ \hat{R}_{12} & \hat{R}_{22}\end{pmatrix} = \begin{pmatrix}[R_{11} \mp 2R_{12} + R_{22}] & [R_{12} \mp R_{22}]\\ [R_{12} \mp R_{22}] & [R_{22}]\end{pmatrix},$$

$$\begin{pmatrix}\hat{k}_1\\ \hat{k}_2\end{pmatrix} = \begin{pmatrix}k_1\\ k_2 \pm k_1\end{pmatrix},$$

$$\begin{pmatrix}\hat{c}_1\\ \hat{c}_2\end{pmatrix} = \begin{pmatrix}c_1\\ [k_2c_2 \pm k_1c_1]/[k_2 \pm k_1]\end{pmatrix}.$$

The D_i generators merely replace $\zeta_i \rightarrow -\zeta_i$. This is not a very interesting transformation since one can always take $\theta \begin{bmatrix}\mathbf{0}\\ \mathbf{0}\end{bmatrix}$ or $\theta \begin{bmatrix}\mathbf{0}\\ \mathbf{1}\end{bmatrix}$, whichever is convenient, as the theta function by adjusting the phase factors ϕ_j in (1.1). These theta functions are always even in each of $\zeta_1,\zeta_2,\ldots,\zeta_N$, so the transformation described by the N D_i invariably leaves the theta function unaltered and is physically irrelevant. Consequently, the only interesting nontrivial transformations are those generated by the smaller set of the $2N^2 - 2N$ matrices that Rauch and Farkas label ${}^{+}A_{ij}$ and ${}^{-}A_{ij}$.

Rauch and Farkas[5] prove that $\mathbf{T}$ is a theta matrix, i.e., symmetric and positive definite imaginary, for the general modular transformation of any N, so the transformed theta function series is always convergent. Although the determinant of $\mathbf{T}$ is invariant under transformation (proof: $\det \mathbf{A}_i = 1$ for all i and the determinant of the product of two arbitrary matrices is the product of their determinants), the trace of $\mathbf{T}$, i.e., the sum of the diagonal elements, generally is altered by the transformation as evident in Table I. Since the trace of the theta matrix is the sum of the eigenvalues, it follows that the eigenvalues, and therefore the rate of convergence of the series are normally changed by the special modular transformation even though the fact of convergence (does it converge or diverge?) is never altered.

These matrices ${}^{\pm}A_{ij}$ exist only for $N \geqslant 2$, i.e., for the double cnoidal wave or higher. All modular transformations for the ordinary cnoidal wave ($N = 1$) yield a result in which the spatial coordinate has both real and imaginary parts except the Poisson summation discussed in the author's earlier paper.[1] In the next section, the simplest nontrivial case $N = 2$ will be described and its generators will be given explicitly.

IV. THE SPECIAL MODULAR TRANSFORMATION FOR $N = 6$: DOUBLE CNOIDAL WAVE

In Rauch and Farkas[5] terminology, there are four generators for $N = 2$, but since half of these are inverses of the other half, there are only two generators[7] in the usual terminology of group theory where inverses are not counted, i.e.,

$$A_1 = \begin{pmatrix}1 & 1\\ 0 & 1\end{pmatrix}, \tag{4.1}$$

$$A_2 = \begin{pmatrix}1 & 0\\ 1 & 1\end{pmatrix}. \tag{4.2}$$

[The inverses are obtained by merely changing the sign of the off-diagonal element for both (4.1) and (4.2).] From Table I, it is apparent that the transformations wrought by A_1 can be obtained from those created by A_2 by interchanging the X and Y coordinates and the subscripts on the theta matrix elements: there is effectively only a single transformation (and its inverse) which can, however, be applied to replace either X or Y by the sum $(X \pm Y)$.

In the companion papers by Boyd,[1] it was convenient to work in terms of modified theta matrices whose elements are denoted by T_{ij} and R_{ij}. Since,

$$T_{ij} \equiv \pi \, \mathrm{Im}(t_{ij}) \tag{4.3}$$

the T_{ij} transform exactly as the complex elements t_{ij} used by mathematicians and vice versa.

The matrix elements R_{ij}, which give the coefficients of the Gaussian series of the theta function, are those of a matrix $\mathbf{R}$ which is proportional to the inverse of $\mathbf{T}$. When $\mathbf{T} \rightarrow \hat{\mathbf{T}} = \mathbf{A}\mathbf{T}\mathbf{A}^T$, the corresponding matrix $\mathbf{R} = (2\pi^2)\ \mathbf{T}^{-1}$ transforms as

$$\hat{\mathbf{R}} = [\mathbf{A}^T]^{-1}\, \mathbf{R}\mathbf{A}^{-1}. \tag{4.4}$$

Equation (4.4) applies for the special modular transformation of any N; the transformed R for the special case $N = 2$ are also given in Table I.

Recalling that $X = k_1\ (x - c_1 t) + \phi_1$ and $Y = k_2\ (x - c\, t) + \phi_2$, it follows that the phase speeds and wavenumbers are also altered by the transformation. The changes made by the generators and their inverses are given in Table I.

V. THE BRANCHING OF THE DISPERSION RELATION

As shown in the Introduction, the existence of the modular transformation implies that each mode of the 2-polycnoidal wave can be transformed into a theta function with $k_1 = 1, k_2 = 2$. This suggests that the dispersion relation for any given set of parameters is infinitely multibranched. At a minimum, it has been shown that if we attempt to make a contour plot of c_1, c_2, and t_{12} for a single mode, say the gravest, then all the higher modes, which are countably infinite in number, provide extraneous roots of the dispersion relation for at least some values of the parameters.

Two issues remain. First, when $k_1 = 1$ and $k_2 = 2$, for example, does the [1,3] mode give a solution of the implicit dispersion relation for all values of (t_{11}, t_{22}) or only for some limited region in parameter space? It is reasonable to conjecture that the correct answer is "all" since the modular transformation is not subject to any parametric restrictions: The transform of a theta function is always a uniformly convergent series of proper theta function form. However, the transformed values of the diagonal theta matrix elements depend on the off-diagonal elements which unfortunately are part of the solution of the dispersion relation, so this conjecture cannot be proved without deeper analysis than that done here.

The second issue is whether all solutions of the implicit dispersion relation are "regular," that is to say, are modes which have well-defined limits for small and large amplitude. Here again, one is tempted to speculate that the answer is that all solutions are regular. The N-polycnoidal waves have an analytic structure which is extraordinarily tidy and simple in other respects. Furthermore, as shown by Boyd,[1] the implicit dispersion can be solved by perturbation theory for both small and large amplitude with good overlap between the two regimes; the overlap implies it is difficult to insert irregular modes that exist only for intermediate parameter values. However, these are not proofs but plausibility arguments. It is known that at least one physically important type of solitary wave, the "modon" of Stern, Flierl, McWilliams, Larichev, and Reznik,[9] does not have a small amplitude limit, but exists only when the amplitude is above some threshold.

Thus, a full resolution of these two issues must remain for future research. It is certain, however, that the implicit dispersion relation for N-polycnoidal waves has multiple solutions for $N \geqslant 2$.

VI. THE WAVENUMBER PARADOX AND THE CONTINUATION METHOD

A good numerical procedure for tracing the structure of a mode is the so-called "continuation" method. The basic idea is to vary one or more of the parameters in small steps. At each step, the algebraic equations are solved for the unknowns via Newton's method. The first guess which is needed to initialize the Newton iteration is obtained by using the results from the previous point in parameter space (or by linear extrapolation from the results at the two previous points); this will always give convergence if the steps in the parameter are sufficiently small. To initialize the parameter march, one needs to know the approximate solution at some point in parameter space. The perturbation theory of Boyd[1] provides such approximate solutions for both very large and very small amplitudes i.e., for very large and small values of t_{ii}, so the continuation method can be easily applied to all the regular solutions of the implicit dispersion relation.

The "paradox of the wavenumbers" is that the gravest mode in the near-soliton limit is $\{1,1\}$, i.e., has $k_1 = k_2 = 1$ while the lowest mode in the small amplitude regime is denoted [1,2] because $k_2 = 2k_1 = 2$. When the continuation method is applied to the $\{1,1\}$ mode, beginning in the large amplitude, near-soliton regime, and both diagonal theta matrix elements are simultaneously increased, what does the algorithm give when $|t_{ii}| \gg 1$? This limit is the small amplitude regime where a mode that is [1,1], i.e., the sum of two sine waves of different phase speeds but identical wavenumbers, cannot exist. Table II answers this question: The continuation method, applied with $k_1 = k_2 = 1$, gives values for c_2 which are the modular transform of those for the gravest small amplitude mode [1,2].

The top line of the table shows the near-soliton regime; the $|t_{ii}|$ are fairly small and the "Gaussian," large amplitude perturbation theory[1] is quite accurate. By the time the bottom is reached, we are in the small amplitude regime and the Gaussian perturbation theory is inaccurate while perturbation theory beginning with two Fourier components as the lowest approximation gives excellent results. However, the continuation method gives $c_2 = -28\pi^2$ in the limit whereas $\cos(2\pi[x - c_1 t])$ and $\cos(4\pi[x - c_2 t])$ have small-amplitude phase speeds of $-4\pi^2$ and $-16\pi^2$, respectively.

TABLE II. Numerical solutions of the residual equations, obtained through the "continuation"method, are compared with zeroth-order Fourier perturbation theory (linear sine waves) and Gaussian perturbation theory (two solitary waves). The percentages are the relative errors. The wavenumbers k_1 and k_2 for the numerical and solitary wave calculations are both equal to 1; $k_2 = 2$ for the Fourier series approximation. The variable c_2^{mod} $(= [c_1 + c_2]/2)$ is the second phase speed after a modular transformation via the generator matrix A_2. This transformation leaves c_1 and k_1 unchanged, but it alters k_2 from 1 to 2.

T_{11}	T_{22}	c_1	c_2	c_2^{mod}	c_1 error	c_2 error
0.8	1.6	313.16	− 402.08	− 44.46		
	(Gaussian)	313.15	− 402.06		9.E-6	6.E-5
	(Fourier)	− 39.48		− 157.92	893.23%	71.84%
1.2	2.4	73.30	− 342.29	− 134.49		
	(Gaussian)	73.31	− 341.68		0.02%	0.18%
	(Fourier)	− 39.48		− 157.91	205.67%	14.83%
1.6	3.2	4.17	− 308.46	− 152.14		
	(Gaussian)	4.27	− 305.72		2.42%	0.89%
	(Fourier)	− 39.48		− 157.91	89.44%	3.65%
2.0	4.0	− 21.14	− 291.40	− 156.27		
	(Gaussian)	− 20.61	− 285.52		2.53%	2.02%
	(Fourier)	− 39.48		− 157.91	46.45%	1.04%
2.4	4.8	− 31.49	− 283.25	− 157.37		
	(Gaussian)	− 29.61	− 274.83		5.97%	2.97%
	(Fourier)	− 39.48		− 157.91	20.25%	0.35%
2.8	5.6	− 35.94	− 279.48	− 157.71		
	(Gaussian)	− 31.11	− 270.65		13.44%	3.16%
	(Fourier)	− 39.48		− 157.91	8.97%	0.13%
3.2	6.4	− 37.90	− 277.76	− 157.83		
	(Gaussian)	− 27.75	− 272.01		26.76%	2.07%
	(Fourier)	− 39.48		− 157.91	4.01%	0.05%

Agreement comes only after making a modular transformation that converts the theta function representation from one with $k_2 = 1$ to $k_2 = 2$, which is the actual wavenumber of one of the two dominant components of this mode in this limit of $|t_{ii}| \to \infty$.

It is useful to see explicitly how a mode can thus diguise itself. The lowest four terms of the Fourier series of the theta function are (in any representation)

$$\theta = 1 + e^{-T_{11}} \cos(2\pi X) + e^{-T_{22}} \cos(2\pi Y) + e^{-T_{11} - T_{22} - 2T_{12}} \cos(2\pi[X + Y]), \tag{6.1}$$

where

$$X = k_1(x - c_1 t), \quad Y = k_2(x - c_2 t). \tag{6.2}$$

The author's companion paper on perturbation theory[1] shows how to evaluate the phase speeds and T_{12} in the "physical" representation $[1,2]^P$; the results are compared against c_1 and c_2^{mod} in Table II. It is also possible, although one would never want to do it except to make a point, to calculate perturbatively in the "unphysical" [1,1] representation as done in Appendix A of that same paper where it is shown that

$$c_1 = -4\pi^2, \tag{6.3}$$

$$c_2 = -28\pi^2, \tag{6.4}$$

$$T_{12} = -T_{11} + \log(3), \tag{6.5}$$

for $T_{11}, T_{22} \gg 1$. Note tht c_2 in (6.4) is the limit of the numerical calculations in Table II for the column labeled "c_2."

In the physical representation $[1,2]^P$, $T_{12} = \log(3)$ and the Fourier series (6.1) is well approximated by the sum of the first three terms. In the "unphysical" [1,1] representation, however, (6.5) shows that the fourth term in (6.1), proportional to $\cos(2\pi[X + Y])$ is larger than the third by a factor $O(e^{T_{11}})$. Discarding $\cos(2\pi Y)$ and taking the double logarithmic derivative gives, using (6.1)–(6.5), the Korteweg–de Vries solution

$$u(x,t) \doteq -48\pi^2(e^{-T_{11}} \cos[2\pi\{x - (-4\pi^2)t\}] + \tfrac{4}{9} e^{-T_{22} + T_{11}} \cos[2\pi\{2x - (-4\pi^2 - 28\pi^2)t\}]). \tag{6.6}$$

The second term in (6.6) travels at a phase velocity of $-16\pi^2$; it is just the expected second harmonic with $k_2 = 2$. In the [1,1] representation, this term appears in disguise as $\cos(2\pi[X + Y])$ [as opposed to $\cos(2\pi Y)$ in the physical $[1,2]^P$ representation], but this disguise cannot change its physical nature.

In the limit of small amplitude, the $N = 2$ Fourier series for $u(x,t)$ is always dominated by just two terms, but the terms wear different disguises in different representations. The second harmonic is $\cos(2\pi[X + Y])$ in the [1,1] representation, $\cos(2\pi Y)$ in the $[1,2]^P$, $\cos(2\pi[-X + Y])$ in the [1,3], and so on.

The moral of the story is that while one can legitimately solve the dispersion relation using any of the infinite number of disguises for a mode which are allowed by the special modular transformation, there is in general only one representation for which the c_1 and c_2 are the actual rates at which components of the 2-polycnoidal wave are traveling. Identifying this "natural" or "physical" representation is clearly an important issue and is therefore the theme of the next section. Table II also shows that the $\{1,1\}$ and [1,2] modes are indeed the same, but the equivalence of these two different disguises of the gravest mode of the 2-polycnoidal wave is obvious only through the modular transformation.

VII. THE CANONICAL OR "PHYSICAL" REPRESENTATION

Because of the freedom provided by the special modular transform, each N-polycnoidal wave for $N \geqslant 2$ can wear a countable infinity of diguises. It follows that a major issue is to identify what representation, i.e., what set of wavenumbers k_1 and k_2, give the "physical" representation in which the wavenumbers and phase speeds directly describe the wave.

We will assert, and then demonstrate below, that the following descriptions of the "physical" or canonical representation are equivalent.

(i) It is the representation in which the phase speeds c_1 and c_2 give the actual average rates of travel of the solitons or sine waves.

(ii) It is the representation which the perturbation series of Boyd[1] calculate in, i.e., the perturbation methods automatically give phase speeds which are the true average rates at which the wave crests move.

(iii) It is the representation in which (small amplitude) the off-diagonal matrix elements t_{ij} $(i \neq j)$ are very small in absolute value in comparison to the diagonal elements t_{ii} or equivalently (large amplitude) the off-diagonal elements R_{ij} are small in comparison to the diagonal elements of the inverse theta matrix R_{ii}.

The first description is simply a definition of what we mean by a "physical" representation. For sufficiently large or small amplitude, the N-polycnoidal wave reduces to the usual N-soliton solution or to a sum of N sine waves, so this definition of a canonical representation is always unambiguous if we are sufficiently close to one or the other of these limiting cases.

The second description is an obvious consequence of the first because the zeroth-order solutions of the perturbation theory are the limits of infinitely large or small amplitude. Thus, the wavenumbers that appear in the zeroth-order solution always count the number of solitons on the interval or are the actual wavenumbers of the sine waves, and this is not changed by adding the higher-order corrections.

The third description is consequence of the following theorem proved in Rauch and Farkas.[5]

Theorem: When the theta matrix is diagonal, i.e., $t_{ij} = 0$ if $i \neq j$, then the N-dimensional theta function may be written as the product of N one-dimensional theta functions

$$\theta(\zeta_1,\zeta_2\cdots,\zeta_N;\mathbf{T}) = \prod_{i=i}^{N} \theta(\zeta_1,t_{ii}). \tag{7.1}$$

The significance of the theorem is that since $u(x,t)$ is proportional to the logarithm of the theta function, each term in the product in (7.1) will contribute additively to the solution of the Korteweg–de Vries equation:

$$u(x,t) = 12 \sum_{i=1}^{N} \frac{d^2}{dx^2} \ln \theta(\zeta_i,t_{ii}). \tag{7.2}$$

This is precisely the situation which occurs in the limits of very large or very small amplitude: the N-polycnoidal wave reduces to a sum of N solitons or sine waves each with its own wavenumber, phase speed, and amplitude. Equation (7.2) and definition (iii) of the "physical" representation are also consistent with the perturbation theory of Boyd[1]: in the limit that the diagonal theta matrix elements (or inverse theta matrix elements) become very large, the off-diagonal elements, which have finite zeroth-order values, necessarily become small relative to the diagonal elements. Thus, both the limiting behavior of the N-polycnoidal wave together with (7.2) and the perturbation theory show that (iii) is true in the physical representation at least for sufficiently large or small diagonal theta matrix elements.

Strictly speaking, of course, no theta matrix for a Korteweg–de Vries solution is ever exactly diagonal; as shown in Appendix B of Ref. 1, the off-diagonal theta matrix elements are responsible for the phase shifts that occur whenever solitons collide. Still, the basic argument is correct, and it can be reversed to justify definition (ii) from (iii). The implicit assumption of the perturbation series of Boyd[1] is that the order of magnitude of different terms in the series can be determined solely from the diagonal theta matrix elements, which is sensible only if the off-diagonal theta matrix elements are small in comparison as required by (iii). Appendix A of the companion paper[1] on perturbation theory is able to calculate perturbation series in an "unphysical" representation only by assuming the diagonal and off-diagonal matrix elements are of the same magnitude. Although no rigorous proof will be given, the fact that the elements of the special modular transformation are always integers strongly suggest that such a transformation will invariably destroy the smallness of the off-diagonal theta matrix elements relative to the diagonal elements at it does in (6.5) so that this smallness is a unique property of the physical representation.

The only flaw with these three equivalent descriptions of the "physical" representation is that they are all in some way tied to the limiting cases of extremes of amplitude or equivalently, of diagonal theta matrix element size. What does one do for intermediate amplitude?

The mathematical response is to use analytic continuation in the parameters: If a given intermediate amplitude solution is the smooth continuation as the parameters are slowly varied of an infinitesimally small amplitude solution whose physical representation is $[1,2]^P$, then this same description is the physical representation of the intermediate amplitude solution, too. Since there is no ambiguity in the limit, there is no ambiguity in this extended definition either as long as the solution branches are continuous with either infinitesimal or infinite amplitude. Note that we use a superscript "P" to denote that the physical representation of a mode is meant, and not one of the infinite number of other representations allowed by the special modular transformation.

There is a remaining physical ambiguity in that Table II shows that the $[1,2]^P$ and $\{1,1\}^P$ representations both describe the same continuous mode: For intermediate amplitude, is it better to describe the polycnoidal wave as a sum of sine waves or of solitons? The answer is given in Ref. 2: For intermediate values of amplitude or of theta matrix elements, both descriptions, as solitons and as sine waves, are qualitatively and even quantitatively correct, and which is better is a matter of individual preference.

VIII. SUMMARY

Mathematicians have known for at least half a century that the theta functions could be expressed in an infinite number of ways via the so-called "modular transformation." The general modular transformation, however, usually gives complex results even though only real values of the space and time variables x and t are relevant to the theory of the Korteweg–de Vries equation. For the ordinary cnoidal wave, which was discovered eighty years ago, the only noncomplex modular transformation is that single transformation which can alternatively be obtained by taking the Poisson sum of the Fourier series of the theta function. Boyd[2] has already discussed the usefulness of this Poisson sum.

It is shown in this paper, however, that for the N-polycnoidal wave with $N \geqslant 2$, where N is the number of arguments of the theta function, there exists a subgroup of the general transformation which does yield nontrivial real results. This subgroup is labeled the "special" modular transformation and is defined to specifically exclude the Poisson sum, which also gives real-valued results but multiplies the theta function by a Gaussian factor. Only the "special"modular transformation and the Poisson sum are useful in the physics of the Korteweg–de Vries equation.

By specializing the rules for the general transformation given in Rauch and Farkas,[5] the generators of the "special" modular transformation are explicitly constructed for arbitrary N. The two generators and their inverses for $N = 2$ are given in Table I above, which also shows the effects of the transformation on the phase speeds and wavenumbers which appear in the "phase" variable that are the arguments of the theta functions.

Since the "special" modular transformation allows each polycnoidal wave to be expressed in an infinite number of ways, a "physical" representation is defined to be that in which the wavenumbers and phase speeds of the theta function match those of the peaks and troughs of the actual wave. Since different polycnoidal waves are obtained for different (physical) wavenumbers, it is helpful to introduce the notation of writing the wavenumbers in [ ] (when θ is represented by a Fourier series) or { } (Gaussian series) and adding a superscript P when the physical representation is meant.

The importance of the special modular transformation in physical applications of the Korteweg–de Vries equations and its cousins is twofold.

First, it shows that the implicit dispersion relation of Boyd[1] for the phase speeds of the polycnoidal wave has an infinite number of solution branches for a given set of parameters (including a fixed set of wavenumbers) even though there is only a single branch for which the wavenumbers are those of the wave's physical representation. Perturbation theory and the "continuation" method are offered as useful ways of computing the physical branch rather than one of the infinite number of other real solutions permitted by the mathematics.

Second, the branch which is the sum of a simple linear sine wave and its second harmonic, $[1,2]^P$ in the notation introduced here, is the sum of one tall solitary wave and one shorter solitary wave on each periodicity interval in the opposite limit of large wave amplitude. This solitary wave limit is written $\{1,1\}^P$; a large amplitude polycnoidal wave for which the wavenumbers $k_1 = 1$ and $k_2 = 2$ are the physical ones is a solution with three solitary waves on each periodicity interval—two of one height and one of a different size. Thus,

$$[1,2]^P = \{1,1\}^P \tag{8.1}$$

in the sense that this single branch must be expressed using a different set of wavenumbers in different amplitude limits if the phase speeds that appear in its theta function are to match those of the actual troughs and crests of the wave.

The special modular transformation is thus essential to understanding the polycnoidal wave because it allows us to change wavenumbers and phase speeds at will so that for any amplitude, we can make the mathematics reflect the physics. Numerically solving the residual equations for fixed wavenumbers, for example, $k_1 = 1$ and $k_2 = 2$, will always give us phase speeds to insert into the theta functions. When we have passed from small wave amplitude to large, however, the phase speeds of the theta functions have only mathematical significance, and differ radically from the actual rates at which the two solitary waves of the branch indicated in (8.1) are traveling, unless we use the special modular transformation to alter the second wavenumber to $k_2 = 1$.

For the Korteweg–de Vries equation and many other soliton equations which are real valued, the special modular transformation (and the Poisson sum discussed in Refs. 1 and 2) are the whole story. Other soliton equations like the cubic Schrödinger equation, however, are intrinsically complex. It is no longer obvious that we should reject the complex-valued transformations which belong to the general modular group but not to the special subgroup defined and constructed here. Future work should explore the physical significance of the general modular transformation for the cubic Schrödinger equation and its complex-valued cousins.

Note added in proof: H. Segur and A. Finkel (unpublished preprint) have applied two-dimensional theta functions and the modular transformation to the Kadomtsev–Petviashvili equation (two space dimensions but only a single phase speed). Their concept of a "basic" theta matrix is an attempt to remove the ambiguity allowed by the modular transformation; in the limits of large and small amplitude, at least, their "basic" matrix is that of the "physical" representation defined here. An earlier work on this same equation (with H. Philander) is "Nonlinear Phenomena" in *Lecture Notes in Physics*, No. 189, edited by K. B. Wolf (Springer-Verlag, Berlin, 1983).

ACKNOWLEDGMENTS

I wish to thank Professor Stanley Jacobs for helpful discussions.

This work was supported by the National Science Foundation through grants OCE 8108530 and OCE 8305648.

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On an extension of the classical Thirring model

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(Received 22 April 1983; accepted for publication 11 May 1984)

A new class of classical field theories, in 1 + 1 dimensions, is introduced, of the form $i\gamma^\mu\Psi_{,\mu} - m\Psi - \bar{\Psi}\gamma^\mu(g_1 + g_2\gamma^5)\Psi\gamma_\mu\Psi - \bar{\Psi}(g_3 + g_4\gamma^5)\Psi\Psi = 0$. It is shown that these theories are relativistically invariant; they do not, however, preserve parity in general, and thus could be used to describe the dynamics of weak interaction processes. The prolongation structure method is used to investigate the existence of pseudopotentials. When the coupling constants g_3 and g_4 are zero, the corresponding theory is then characterized by an infinite family of conservation laws and is thus completely integrable. For this very case, the Bäcklund map (pseudopotential) furnishes the equivalent of a Lax pair of operators as well as a nontrivial Bäcklund transformation and solutions of soliton type.

PACS numbers: 02.30.Jr, 03.50.Kk

I. INTRODUCTION

Since a decade or so, nonlinear systems (of partial differential equations) brought a new interest in the physics community. Indeed, such systems present new kinds of solutions, e.g., solitons, which behave in a radically different manner than solutions of linear systems. These objects have direct physical interpretations in many different contexts. One may consider, for instance, the importance of the soliton solutions of the well-known sine–Gordon equation in regard of the dynamical behavior of ultrashort laser pulses, those of the nonlinear cubic Schrödinger equation in nonlinear optics, or the role played in hydrodynamics by the Korteweg–de Vries, Kadomtsev–Petviashvili, and Benjamin–Ono equations.

The purpose of this article is to propose and study a model of classical field theory, defined in 1 + 1 space-time dimensions, generalizing the classical massive Thirring model.[1] Like the Thirring model, the proposed one represents the self-interaction of a spinor particle. The requirements of parity and time-reversal invariance are dropped (a quantized version of it could therefore be used to describe a weak self-interaction), hence the self-interaction can have a more general form [see (2.1) below].

The Thirring model was initially proposed in 1958 and its original interest was in that it provided a solvable model of a nonlinear quantum field theory. The basic equations of the classical version of that model are

$$i\gamma^\mu\Psi_{,\mu} - m\Psi - g\bar{\Psi}\gamma^\mu\Psi\gamma_\mu\Psi = 0, \tag{1.1}$$

where

$$\gamma^0 = \gamma_0 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \gamma^1 = -\gamma_1 = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$
$$\gamma^5 = -\gamma_5 = \gamma^0\gamma^1 = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix},$$

and $\bar{\Psi} = \Psi^\dagger\gamma^0, \Psi_{,\mu} = \partial\Psi/\partial x^\mu$. The quantum theory built around this equation raised many polemics in its early history and revealed itself to be somewhat tricky.[2] It was later shown that (1.1) possesses soliton solutions which can be constructed, for example, from the soliton solutions of the sine–Gordon equation via so-called Coleman's correspondences.[3,4] Considered in a purely classical scheme, the model also accepts solitons as solutions and a particularly nice way to obtain them is by using the prolongation method devised by Wahlquist and Estabrook.[5,6] It is known that their procedure is quite rich in content.[7–9] Indeed its central result, Bäcklund maps (or, equivalently, pseudopotentials) may yield several secondary results such as conservation laws, solitons, and linear equations that can be used as a starting point for an inverse scattering transform problem.

The outline of the present article is as follows. In Sec. II, we introduce a general model and establish its Poincaré invariance. In Sec. III, we literally apply the prolongation method. To this end, it is convenient to replace the differential system by an equivalent Pfaffian system of two-forms. We then reset the integrability conditions into a set of commutation relations on operators lying in a Lie algebra which we shall choose to be sl (2,ℂ). To each solution of that set corresponds a Bäcklund map and the family of these will provide us with a classification of submodels with respect to subalgebras of sl (2,ℂ). When the whole algebra is involved, we observe that the Bäcklund map contains a free parameter which proves to be important since it characterizes the very case for which the most interesting results are obtained. The search for Bäcklund transformations is the object of Sec. IV and there again it is seen that the free parameter is essential in order to obtain a nontrivial transformation. In Sec. V, we shall find solutions of soliton type for the nontrivial case with the help of the Bäcklund transformation found in the preceding section. Finally, Sec. VI will be devoted to conclusions; we shall give a summary as well as an outlook on certain as yet unanswered questions directly related to the subject of this article.

II. A GENERALIZED THIRRING MODEL

Let us begin by introducing some of the basic notation that we shall use throughout our investigation. The space of independent variables will be the usual Minkowski's manifold M with local coordinate functions $\{x^0 = t, x^1 = x\}$ or $\{2\xi = t + x, 2\eta = t - x\}$, and metric tensor

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$$g=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}.$$

We define a field Ψ with components ψ_1,ψ_2 as a $M\to\mathbb{C}^2$ mapping. Notice that the components can also be thought of as local coordinate functions on a manifold N (the space of dependent variables), and we may thus define the first jet bundle $J^1(M,N)$ with local coordinate functions $\{x^\mu;\psi_i,\ \psi_{i,\mu}=\partial\psi_i/\partial x^\mu\}$. We shall follow Einstein's summation convention on repeated indices. Finally, all constants will be considered real unless they are explicitly defined as complex quantities.

Examining (1.1), we notice that it is characterized by a nonlinear part made of a single trilinear form in the fields: certainly, this is not exhaustive. We shall therefore generalize the system by implementing (1.1) with a more general linear combination of trilinear forms. The most general one is easily seen to take the form

$$i\gamma^\mu\Psi_{,\mu}-m\Psi-\bar\Psi\gamma^\mu(g_1+g_2\gamma^5)\Psi\gamma_\mu\Psi-\bar\Psi(g_3+g_4\gamma^5)\Psi\Psi=0 \tag{2.1}$$

or, in component form,

$$\begin{aligned} &i\psi_{2,\xi}-m\psi_1-b_0|\psi_1|^2\psi_2-c_0\psi_1^2\bar\psi_2=0,\\ &i\psi_{1,\eta}-m\psi_2-b_1|\psi_2|^2\psi_1-c_1\psi_2^2\psi_1=0,\end{aligned} \tag{2.2}$$

where

$$b_0=2(g_1-g_2)+c_1,\quad c_0=g_3-g_4,$$
$$b_1=2(g_1+g_2)+c_0,\quad c_1=g_3+g_4.$$

Here, $\bar\psi_i$ stands for the complex conjugate of ψ_i.

Remark: As will be seen later on, the sole subsystem of (2.1) that will yield nontrivial results is the one for which $g_3=g_4=0$, i.e., when we restrict ourselves to current-pseudocurrent types of interactions. It might therefore be more appropriate to refer to this very subsystem as the "extended Thirring model."

Lie symmetries of the system (2.1) can be found quite easily. Let us first rewrite this system in the form

$$i\gamma^\mu\Psi_{,\mu}-m\Psi\equiv D\Psi=f(\Psi),$$

and introduce an infinitesimal Lie vector field

$$X=a^\nu(t,x)\partial_\nu+c(t,x), \tag{2.3}$$

where the a^ν's are real functions and c a possibly complex function. As it is well known, the symmetries of (2.1) are obtained by requiring that the following Fréchet derivative vanishes identically:

$$D'(\Psi)[X]=0. \tag{2.4}$$

Using (2.3) and subtracting a term $XD\Psi=Xf(\Psi)$, (2.4) can be rewritten as the commutator relation

$$[D,X]=f(X\Psi)-Xf(\Psi).$$

Replacing D and f by their explicit expressions, this is then easily solved for X. We find

$$\begin{aligned} X&=(2\lambda x+\sigma^0)\partial_t+(2\lambda t+\sigma^1)\partial_x+(i\omega-\lambda\gamma^5)\\ &=\lambda M+\sigma^0P_0+\sigma^1P_1+\omega E,\end{aligned}$$

where $\lambda,\sigma^0,\sigma^1,\omega$ are real parameters. It is then clear that (2.1) is invariant under a group $P(1,1)\times U(1)$, where $P(1,1)$ is the usual two-dimensional Poincaré group.

Now, as fas as discrete symmetries are concerned, it is also clear that (2.1) has generally none save the trivial one. However, if we set $g_2=g_4=0$ or $g_1=g_3=0$, the resulting subsystems are invariant under parity inversion and time reversal, respectively.

III. THE PROLONGATION STRUCTURE AND EXISTENCE OF PSEUDOPOTENTIALS

Let us return to Eq. (2.2) and their complex conjugates. These form a set of four equations which defines a differential system $Z\subset J^1(M,\mathbb{C}^2)$, where $J^1(M,\mathbb{C}^2)$ is described with coordinate functions $\{x^\mu;\psi_i,\bar\psi_i,\psi_{i,\mu},\bar\psi_{i,\mu}\}$, with domain M, range $\mathbb{C}^2$, and order one. In other words, it is the zero set of the ideal I_Z of functions on $J^1(M,\mathbb{C}^2)$ generated by

$$\begin{aligned} F_1&=i\psi_{2,\xi}-m\psi_1-b_0|\psi_1|^2\psi_2-c_0\psi_1^2\bar\psi_2,\\ F_2&=i\psi_{1,\eta}-m\psi_2-b_1|\psi_2|^2\psi_1-c_1\psi_2^2\bar\psi_1,\\ F_3&=i\bar\psi_{2,\xi}+m\bar\psi_1+b_0|\psi_1|^2\bar\psi_2+c_0\bar\psi_1^2\psi_2,\\ F_4&=i\bar\psi_{1,\eta}+m\bar\psi_2+b_1|\psi_2|^2\bar\psi_1+c_1\bar\psi_2^2\psi_1.\end{aligned} \tag{3.1}$$

Moreover we notice that Z is a quasilinear-type nonlinear differential system. This is enough to ensure that Z can be replaced by an exterior differential (Pfaffian) system I_Z on $J^0(M,\mathbb{C}^2)\sim M\times\mathbb{C}^2$ which has exactly the same solution space as that of Z. It is found that I_Z is the closed (differential) ideal on $J^0(M,\mathbb{C}^2)$ generated by

$$\begin{aligned} \omega^1&=i\,d\psi_1\wedge d\xi+(m\psi_2+b_1|\psi_2|^2\psi_1+c_1\psi_2^2\bar\psi_1)d\xi\wedge d\eta,\\ \omega^2&=i\,d\psi_2\wedge d\eta-(m\psi_1+b_0|\psi_1|^2\psi_2+c_0\psi_1^2\bar\psi_2)d\xi\wedge d\eta,\\ \omega^3&=i\,d\bar\psi_1\wedge d\xi-(m\bar\psi_2+b_1|\psi_2|^2\bar\psi_1+c_1\bar\psi_2^2\psi_1)d\xi\wedge d\eta,\\ \omega^4&=i\,d\bar\psi_2\wedge d\eta+(m\bar\psi_1+b_0|\psi_1|^2\bar\psi_2+c_0\bar\psi_1^2\psi_2)d\xi\wedge d\eta,\\ \sigma^{i\nu}&=d\psi_i\wedge dx^\nu-\psi_{i,\mu}dx^\mu\wedge dx^\nu,\\ \bar\sigma^{i\nu}&=d\bar\psi_i\wedge dx^\nu-\bar\psi_{i,\mu}dx^\mu\wedge dx^\nu.\end{aligned}$$

Thus any $f\in\Gamma(M,\mathbb{C}^2)$ (i.e., the set of all $U\subset M\to\mathbb{C}^2$ mappings) is a solution of Z iff $(j^1f)^*I_Z=0$. Let us now apply the method of Wahlquist and Estabrook. First, we have to choose a closed proper subideal $I'_Z\subset I_Z$. We may select the one generated by $\{\omega^i\}_1^4$ which, clearly, satisfies those requirements. Our interest is to construct a Bäcklund map (not to be confused with a Bäcklund transformation as it will be defined in the next section[10]) for the system Z defined by (3.1). To this end, we introduce a mapping $\chi:J^1(M,\mathbb{C}^2)\times\mathbb{C}^n\to J^1(M,\mathbb{C}^n)$ preserving the local charts on M and $\mathbb{C}^n$, and having the (partial) local representation

$$y^A{}_{,\mu}=\chi^A{}_{,\mu}(\psi_i,\bar\psi_i,\psi_{i,\nu},\bar\psi_{i,\nu};y^B),$$

where $1\leqslant A,B\leqslant n$ and $\mu,\nu=0,1$. For reasons of simplicity, we shall assume no explicit dependence on the independent variables $\{x^\mu\}$ nor on $\{\overline{y^B}\}$. In order to completely determine χ, we must now ensure that its integrability conditions are equivalent to the initial equation (2.2). This will actually be so if

$$\chi^*\,d\Omega^1(M,\mathbb{C}^n)\subset I(\Omega^2(\chi)), \tag{3.2}$$

where

$$I(\Omega^2(\chi)) = \{\Sigma\eta_i \wedge \omega^i | \omega^i \in \Omega^2(\chi) \text{ and } \eta_i \text{ is any form}\},$$
$$\Omega^2(\chi) = \Omega^2(M,\mathbb{C}^2) + \Omega^1(M,\mathbb{C}^n),$$

and

$$\Omega^k(M,N) = \{\theta \in \Lambda^1(J^k(M,N)) | (j^k f)^* \theta = 0\}.$$

For the sake of a compact notation, notice that we made the following identifications:

$$\chi \sim \tilde{\pi}_1^{2*}\chi, \quad \Omega^1(M,\mathbb{C}^n) \sim \tilde{\pi}_1^{2*}\chi \, {}^*\Omega^1(M,\mathbb{C}^n),$$
$$\Omega^2(M,\mathbb{C}^2) \sim S_1^*\Omega^2(M,\mathbb{C}^2),$$

where $S_1 : J^1(M,\mathbb{C}^2)\times\mathbb{C}^n \to J^1(M,\mathbb{C}^2)$ is the canonical projection on the first factor, and

$$\tilde{\pi}_1^2 : J^2(M,\mathbb{C}^2)\times\mathbb{C}^n \to J^1(M,\mathbb{C}^2)\times\mathbb{C}^n : (j_x^2 f, p) \mapsto (j_x^1 f, p).$$

But how does (3.2) translate in local terms? Let $\Omega^1(M,\mathbb{C}^n)$ have the basis $\{\theta^A = dy^A - y^A{}_{,\mu}\, dx^\mu \mid 1 \leqslant A \leqslant n\}$. Writing $\chi^* \theta^A = dy^A - \chi^A{}_{,\mu}\, dx^\mu$ and $d\chi^* \theta^A = -d\chi^A{}_{,\mu} \wedge dx^\mu$, (3.2) is then equivalent to the strict requirement that, for any A, $-d\chi^A{}_{,\mu} \wedge dx^\mu$ should be a linear combination of the $\{\omega^i\}_1^4$ and of the $\{\chi^* \theta^A\}$ (under exterior differentiation):

$$d\chi^A{}_{,\mu} \wedge dx^\mu + H_i{}^A \omega^i + (K^A{}_{BC} dy^B + M^A{}_{C\mu}\, dx^\mu) \wedge (dy^C - \chi^C{}_{,\nu} dx^\nu) = 0,$$

where the $\{H_i{}^A, K^A{}_{BC}, M^A{}_{C\mu}\}$ are functions. We expand this explicitly and, using the linear independence between the basis forms, we show that it is equivalent to the following requirements:

$$y^A{}_{,\xi} = \chi^A{}_{,\xi}(\psi_1, \bar{\psi}_1; y^B), \quad y^A{}_{,\eta} = \chi^A{}_{,\eta}(\psi_2, \bar{\psi}_2; y^B), \tag{3.3}$$

and

$$\begin{aligned}[\hat{\chi}_{,\xi}, \hat{\chi}_{,\eta}] = &- i\hat{\chi}_{,\xi\psi_1}(m\psi_2 + b_1|\psi_2|^2\psi_1 + c_1\psi_2^2\bar{\psi}_1) \\ &+ i\hat{\chi}_{,\eta\psi_2}(m\psi_1 + b_0|\psi_1|^2\psi_2 + c_0\psi_1^2\bar{\psi}_2) \\ &+ i\hat{\chi}_{\xi\bar{\psi}_1}(m\bar{\psi}_2 + b_1|\psi_2|^2\bar{\psi}_1 + c_1\bar{\psi}_2^2\psi_1) \\ &- i\hat{\chi}_{,\eta\bar{\psi}_2}(m\bar{\psi}_1 + b_0|\psi_1|^2\bar{\psi}_2 + c_0\bar{\psi}_1^2\psi_2),\end{aligned} \tag{3.4}$$

where $\hat{\chi} = \chi^A \partial/\partial y^A$. Can we integrate this? Using (3.3) and computing the successive partial derivatives of (3.4) with respect to the dependent variables $\psi_i, \bar{\psi}_i$, we obtain the following results:

$$\frac{\partial^2}{\partial p\, \partial q}[\hat{\chi}_{,\xi\psi_1\bar{\psi}_1}, \hat{\chi}_{,\eta\psi_2\bar{\psi}_2}] = 0, \tag{3.5}$$

where $(p,q) \in \{\psi_1, \bar{\psi}_1\} \times \{\psi_2, \bar{\psi}_2\}$. We shall now make the following simplifying assumption: let us demand that $\hat{\chi}_{,\xi}$ and $\hat{\chi}_{,\eta}$ lie in the Lie algebra sl (2,C). Considering sl (2,C) as a three-dimensional complex Lie algebra, we know that $[X_1, X_2] = 0$ implies either that (a) one or both of the X_i's are zero, or that (b) one of the X_i's is proportional to the other. Using this fact with (3.5), and (3.4) again, we deduce that the most general expressions for $\hat{\chi}_{,\xi}$ and $\hat{\chi}_{,\eta}$ are

$$\begin{aligned}\hat{\chi}_{,\xi} = &\hat{P}_0 + \psi_1\hat{P}_1 + \bar{\psi}_1\hat{P}_2 + \psi_1^2\hat{P}_3 + |\psi_1|^2\hat{P}_4 \\ &+ \bar{\psi}_1^2\hat{P}_5 + |\psi_1|^2\psi_1\hat{P}_6 + |\psi_1|^2\bar{\psi}_1\hat{P}_7,\end{aligned} \tag{3.6}$$

$$\begin{aligned}\hat{\chi}_{,\eta} = &\hat{Q}_0 + \psi_2\hat{Q}_1 + \bar{\psi}_2\hat{Q}_2 + \psi_2^2\hat{Q}_3 + |\psi_2|^2\hat{Q}_4 \\ &+ \bar{\psi}_2^2\hat{Q}_5 + |\psi_2|^2\psi_2\hat{Q}_6 + |\psi_2|^2\bar{\psi}_2\hat{Q}_7,\end{aligned}$$

where $\hat{P}_i = P_i{}^A(y^B)\partial/\partial y^A$ and $\hat{Q}_i = Q_i{}^A(y^B)\partial/\partial y^A$.

Remark: It should be noticed, at this point, that the method of Wahlquist and Estabrook yields, in general, infinite-dimensional Lie algebras. Here we imposed a quite drastic closure condition by demanding that $\hat{X}_{,\xi}, \hat{X}_{,\eta} \in$ sl (2,C). Naturally this will imply that the prolongation structure may not be as rich as it could be. Yet, interesting results will still follow.

Our next step is to substitute (3.6) into (3.4). Doing this and using the linear independence of the different powers $\psi_1{}^a\bar{\psi}_1{}^b\psi_2{}^c\bar{\psi}_2{}^d$, (3.4) resumes itself to a set of 64 commutation relations to be solved for the $\hat{P}_i$'s and $\hat{Q}_i$'s. This set can be reduced if we make the following further reasonable assumption: $\hat{Q}_i = \sigma_i\hat{P}_i, \sigma_i \in \mathbb{C}\setminus\{0\}$ [this is motivated by the similarities in (3.6)]. We thus obtain

$$\begin{aligned}
&[\hat{P}_0,\hat{P}_1] = -im\hat{P}_1/\sigma_1 = -im\sigma_1\hat{P}_1/\sigma_0, \\
&[\hat{P}_0,\hat{p}_2] = im\hat{P}_2/\sigma_2 = im\sigma_2\hat{P}_2/\sigma_0, \\
&[\hat{P}_1,\hat{P}_2] = im(1+\sigma_4)\hat{P}_4/\sigma_2 = im(1+\sigma_4)\hat{P}_4/\sigma_1, \\
&[\hat{P}_1,\hat{P}_4] = -ib_1\hat{P}_1/\sigma_4 + 2im\sigma_6\hat{P}_6/\sigma_4 \\
&\qquad = -ib_0\hat{P}_1 + 2im\hat{P}_6/\sigma_1, \\
&[\hat{P}_1,\hat{P}_5] = ic_1\hat{P}_2/\sigma_3 + im\sigma_7\hat{P}_7/\sigma_5 \\
&\qquad = ic_0\sigma_2\hat{P}_2/\sigma_1 + im\hat{P}_7/\sigma_1, \\
&[\hat{P}_2,\hat{P}_3] = -ic_1\hat{P}_1/\sigma_3 - im\sigma_6\hat{P}_6/\sigma_3 \\
&\qquad = -ic_0\sigma_1\hat{P}_1/\sigma_2 - im\hat{P}_6/\sigma_2, \\
&[\hat{P}_2,\hat{P}_4] = ib_1\hat{P}_2/\sigma_4 - 2im\sigma_7\hat{P}_7/\sigma_4 \\
&\qquad = ib_0\hat{P}_2 - 2im\hat{P}_7/\sigma_2, \\
&[\hat{P}_3,\hat{P}_4] = 2i(c_0\sigma_3 - b_1)\hat{P}_3/\sigma_4 = 2i(c_1 - b_0\sigma_3)\hat{P}_3/\sigma_3, \\
&[\hat{P}_3,\hat{P}_5] = i(c_0\sigma_4 + c_1)\hat{P}_4/\sigma_5 = i(c_0\sigma_4 + c_1)\hat{P}_4/\sigma_3, \\
&[\hat{P}_4,\hat{P}_5] = 2i(c_1 - b_0\sigma_5)\hat{P}_5/\sigma_5 = 2i(c_0\sigma_5 - b_1)\hat{P}_5/\sigma_4, \\
&[\hat{P}_4,\hat{P}_6] = ib_0\hat{P}_6 = ib_1\hat{P}_6/\sigma_4, \\
&[\hat{P}_4,\hat{P}_7] = -ib_0\hat{P}_7 = -ib_1\hat{P}_7/\sigma_4, \\
&[\hat{P}_0,\hat{P}_3] \\
&\qquad = [\hat{P}_0,\hat{P}_4] = [\hat{P}_0,\hat{P}_5] = [\hat{P}_0,\hat{P}_6] = [\hat{P}_0,\hat{P}_7] = [\hat{P}_1,\hat{P}_3] \\
&\qquad = [\hat{P}_1,\hat{P}_6] = [\hat{P}_1,\hat{P}_7] = [\hat{P}_2,\hat{P}_5] = [\hat{P}_2,\hat{P}_6] = [\hat{P}_2,\hat{P}_7] \\
&\qquad = [\hat{P}_3,\hat{P}_6] = [\hat{P}_3,\hat{P}_7] = [\hat{P}_5,\hat{P}_6] = [\hat{P}_5,\hat{P}_7] = [\hat{P}_6,\hat{P}_7] \\
&\qquad = 0, \\
&m(1-\sigma_3)\hat{P}_3 = m(1-\sigma_5)\hat{P}_5 = 0, \\
&c_0\hat{P}_6 = c_1\hat{P}_6 = c_0\hat{P}_7 = c_1\hat{P}_7 = 0.
\end{aligned} \tag{3.7}$$

We solve this in the following sense. It is not guaranteed *a priori* that Z will possess a Bäcklund map other than the trivial one. Therefore we shall classify all subsystems of Z (defined through restrictions on $\{b_i, c_i\}$) for which there exists a Bäcklund map. In order to do that, the algorithm to use is as follows. First, consider $\hat{P}_0$: it can be either zero or different from zero; both of these alternatives will reduce (3.7) into smaller sets of commutation relations, each with additional constraints on the σ_i's, $\hat{P}_i$'s, b_i's, c_i's (we assume further that $m \neq 0$). We repeat these considerations with $\hat{P}_1$, $\hat{P}_2$, and so forth, up to the point where all of the $\hat{P}_i$'s will be completely determined within the algebra. The result is six classes of subsystems $Z_i \subset Z$, up to complex conjugations and various

affine transformations on the $\{y^A\}$. For a deeper classification, we also used the fact that an arbitrary element of sl (2,$\mathbb{C}$) is a conjugate, under SL (2,$\mathbb{C}$), of either T_2 or αT_0. Here, we chose $\{T_0, T_1, T_2\}$ as the basis of the algebra sl (2,$\mathbb{C}$), with the following defining commutation relations:

$$[T_0,T_1] = iT_1,$$
$$[T_0,T_2] = -iT_2,$$
$$[T_1,T_2] = 2iT_0.$$

We now list representatives from these classes with their corresponding field equations, where

$$\alpha,\delta_i\in\mathbb{C},\quad \epsilon,\sigma\in\mathbb{C}\setminus\{0\},\quad \delta\in\{0,1\},\quad T\in\{T_2,\alpha T_0\};$$

$$\hat{\chi}_{,\xi} = 0,$$
$$\hat{\chi}_{,\eta} = 0,$$
$$i\psi_{2,\xi} = m\psi_1 + (2g_1 - 2g_2 + g_3 + g_4)|\psi_1|^2\psi_2 + (g_3 - g_4)\psi_1^2\bar{\psi}_2, \tag{3.8a}$$
$$i\psi_{1,\eta} = m\psi_2 + (2g_1 + 2g_2 + g_3 - g_4)|\psi_2|^2\psi_1 + (g_3 + g_4)\psi_2^2\bar{\psi}_1;$$

$$\hat{\chi}_{,\xi} = (\delta + |\psi_1|^2)T,$$
$$\hat{\chi}_{,\eta} = (\delta - |\psi_2|^2)T,$$
$$i\psi_{2,\xi} = m\psi_1 + (2g_1 - 2g_2 + g_3)|\psi_1|^2\psi_2 + g_3\psi_1^2\bar{\psi}_2, \tag{3.8b}$$
$$i\psi_{1,\eta} = m\psi_2 + (2g_1 + 2g_2 + g_3)|\psi_2|^2\psi_1 + g_3\psi_2^2\bar{\psi}_1;$$

$$\hat{\chi}_{,\xi} = (\delta_1\psi_1^2 + \delta_2\bar{\psi}_1^2)T,$$
$$\hat{\chi}_{,\eta} = (\delta_1\psi_2^2 + \delta_2\bar{\psi}_2^2)T, \tag{3.8c}$$
$$i\psi_{2,\xi} = m\psi_1 + (g_3 + g_4)|\psi_1|^2\psi_2 + (g_3 - g_4)\psi_1^2\bar{\psi}_2,$$
$$i\psi_{1,\eta} = m\psi_2 + (g_3 - g_4)|\psi_2|^2\psi_1 + (g_3 + g_4)\psi_2^2\bar{\psi}_1;$$

$$\hat{\chi}_{,\xi} = (1 + \delta_1\psi_1^2 + \epsilon|\psi_1|^2 + \delta_2\bar{\psi}_1^2)T,$$
$$\hat{\chi}_{,\eta} = (1 + \delta_1\psi_2^2 - \epsilon|\psi_2|^2 + \delta_2\bar{\psi}_2^2)T, \tag{3.8d}$$
$$i\psi_{2,\xi} = m\psi_1 + g_3|\psi_1|^2\psi_2 + g_3\psi_1^2\bar{\psi}_2,$$
$$i\psi_{1,\eta} = m\psi_2 + g_3|\psi_2|^2\psi_1 + g_3\psi_2^2\bar{\psi}_1;$$

$$\hat{\chi}_{,\xi} = \psi_1^2 T_1 - 4g_2g_4\bar{\psi}_1^2 T_2 + 4g_2|\psi_1|^2T_0,$$
$$\hat{\chi}_{,\eta} = \psi_2^2 T_1 - 4g_2g_4\bar{\psi}_2^2 T_2 - 4g_2|\psi_2|^2T_0, \tag{3.8e}$$
$$i\psi_{2,\xi} = m\psi_1 + (g_3 + g_4 - 2g_2)|\psi_1|^2\psi_2 + (g_3 - g_4)\psi_1^2\bar{\psi}_2,$$
$$i\psi_{1,\eta} = m\psi_2 + (g_3 - g_4 + 2g_2)|\psi_2|^2\psi_1 + (g_3 + g_4)\psi_2^2\bar{\psi}_1;$$

$$\hat{\chi}_{,\xi} = [2(g_1 - g_2)|\psi_1|^2 - m/\sigma]T_0 + \psi_1T_1 - 2mg_1/\sigma\cdot\bar{\psi}_1T_2,$$
$$\hat{\chi}_{,\eta} = [2(g_1 + g_2)|\psi_2|^2 - m\sigma]T_0 + \sigma\psi_2T_1 + 2mg_1\bar{\psi}_2T_2,$$
$$i\psi_{2,\xi} = m\psi_1 + 2(g_1 - g_2)|\psi_1|^2\psi_2, \tag{3.8f}$$
$$i\psi_{1,\eta} = m\psi_2 + 2(g_1 + g_2)|\psi_2|^2\psi_1.$$

We thus have specified all the Bäcklund maps with their corresponding subsystems $Z_i\subset Z$. Here, we shall restrict ourselves to y as being one or two dimensional. With respect to this, consider the following realizations of sl (2,$\mathbb{C}$):

$$T_0 = iy\frac{d}{dy},\quad T_1 = y^2\frac{d}{dy},\quad T_2 = \frac{d}{dy};$$
$$T_0 = -\frac{1}{2}i\left(y_1\frac{\partial}{\partial y_1} - y_2\frac{\partial}{\partial y_2}\right),$$
$$T_1 = -iy_2\frac{\partial}{\partial y_1},\quad T_2 = -iy_1\frac{\partial}{\partial y_2}.$$

Also consider the corresponding forms for the Bäcklund maps:

$$\hat{\chi}_{,\xi} = y_{,\xi}\frac{d}{dy},\quad \hat{\chi}_{,\eta} = y_{,\eta}\frac{d}{dy};$$
$$\hat{\chi}_{,\xi} = y_{1,\xi}\frac{\partial}{\partial y_1} + y_{2,\xi}\frac{\partial}{\partial y_2},\quad \hat{\chi}_{,\eta} = y_{1,\eta}\frac{\partial}{\partial y_1} + y_{2,\eta}\frac{\partial}{\partial y_2}.$$

Explicitly, (3.8) gives the following one- and two-dimensional maps (3.9) and (3.10), respectively. For the two-dimensional ones, we use $Y = \left[\begin{smallmatrix} y_1 \\ y_2 \end{smallmatrix}\right]$:

$$y_{,\xi} = 0,\quad y_{,\eta} = 0, \tag{3.9a}$$
$$y_{,\xi} = (\delta + |\psi_1|^2)v,\quad y_{,\eta} = (\delta - |\psi_2|^2)v, \tag{3.9b}$$
$$y_{,\xi} = (\delta_1\psi_1^2 + \delta_2\bar{\psi}_1^2)v,\quad y_{,\eta} = (\delta_1\psi_2^2 + \delta_2\bar{\psi}_2^2)v, \tag{3.9c}$$
$$y_{,\xi} = (1 + \delta_1\psi_1^2 + \epsilon|\psi_1|^2 + \delta_2\bar{\psi}_1^2)v,$$
$$y_{,\eta} = (1 + \delta_1\psi_2^2 - \epsilon|\psi_2|^2 + \delta_2\bar{\psi}_2^2)v, \tag{3.9d}$$
$$y_{,\xi} = \psi_1^2y^2 + 4ig^2|\psi_1|^2y - 4g_2g_4\bar{\psi}_1^2,$$
$$y_{,\eta} = \psi_2^2y^2 - 4ig_2|\psi_2|^2y - 4g_2g_4\bar{\psi}_2^2, \tag{3.9e}$$
$$y_{,\xi} = \psi_1y^2 - i[m/\sigma - 2(g_1 - g_2)|\psi_1|^2]y + 2mg_1/\sigma\cdot\bar{\psi}_1,$$
$$y_{,\eta} = \sigma\psi_2y^2 - i[m\sigma - 2(g_1 + g_2)|\psi_2|^2]y + 2mg_1\bar{\psi}_2, \tag{3.9f}$$

where $v\in\{1, \alpha y\}$;

$$Y_{,\xi} = 0,\quad Y_{,\eta} = 0, \tag{3.10a}$$
$$Y_{,\xi} = (\delta + |\psi_1|^2)VY,\quad Y_{,\eta} = (\delta - |\psi_2|^2)VY, \tag{3.10b}$$
$$Y_{,\xi} = (\delta_1\psi_1^2 + \delta_2\bar{\psi}_1^2)VY,\quad Y_{,\eta} = (\delta_1\psi_2^2 + \delta_2\bar{\psi}_2^2)VY, \tag{3.10c}$$
$$Y_{,\xi} = (1 + \delta_1\psi_1^2 + \epsilon|\psi_1|^2 + \delta_2\bar{\psi}_1^2)VY,$$
$$Y_{,\eta} = (1 + \delta_1\psi_2^2 - \epsilon|\psi_2|^2 + \delta_2\bar{\psi}_2^2)VY, \tag{3.10d}$$
$$Y_{,\xi} = \begin{bmatrix} -2ig_2|\psi_1|^2 & -i\psi_1^2 \\ 4ig_2g_4\bar{\psi}_1^2 & 2ig_2|\psi_1|^2 \end{bmatrix} Y, \tag{3.10e}$$
$$Y_{,\eta} = \begin{bmatrix} 2ig_2|\psi_2|^2 & -i\psi_2^2 \\ 4ig_2g_4\bar{\psi}_2^2 & -2ig_2|\psi_2|^2 \end{bmatrix} Y,$$

$$Y_{,\xi} = \begin{bmatrix} \frac{1}{2}i[m/\sigma - 2(g_1 - g_2)|\psi_1|^2] & -i\sqrt{2mg_1}\psi_1 \\ -i\sqrt{2mg_1}\bar{\psi}_1/\sigma & -\frac{1}{2}i[m/\sigma - 2(g_1 - g_2)|\psi_1|^2] \end{bmatrix} Y, \tag{3.10f}$$

$$Y_{,\eta} = \begin{bmatrix} \frac{1}{2}i[m\sigma - 2(g_1 + g_2)|\psi_2|^2] & -i\sqrt{2mg_1}\sigma\psi_2 \\ -i\sqrt{2mg_1}\bar{\psi}_2 & -\frac{1}{2}i[m\sigma - 2(g_1 + g_2)|\psi_2|^2] \end{bmatrix} Y,$$

where

$$V=\begin{bmatrix} 0 & 0 \\ -i & 0 \end{bmatrix} \quad \text{or} \quad V=\begin{bmatrix} -\frac{1}{2}i\alpha & 0 \\ 0 & \frac{1}{2}i\alpha \end{bmatrix}.$$

Before pursuing any further, let us make a few remarks. It should be noticed that Bäcklund maps may contain free parameters and these may not always be indicative of Lie symmetries of the initial differential system. In particular, it is so for the last case in our classification where the free parameter is σ. There, the relevant symmetry which causes the occurence of σ is rather a symmetry of the prolongation structure, i.e., a symmetry of the ideal $\Omega^2(\chi)$.

Examining (3.9), we observe that the Bäcklund maps are all Riccati-type coupled systems, or restrictions of such systems; this is naturally a consequence of the choice of sl(2,C) as a prolongation algebra. We also observe that for each Bäcklund map the corresponding one-form in $\Omega^1(M,\mathbb{C})$ can be written as

$$\theta = dy - y_{,\xi}\, d\xi - y_{,\eta}\, d\eta = dy - \omega_0 - \omega_1 y - \omega_2 y^2.$$

Since our basis for sl (2,C) was chosen to be $\{d/dy, iyd/dy, y^2 d/dy\}$, we readily see that any such one-form defines a SL(2,C) connection of Cartan–Ehresmann type in the fiber bundle $J^1(M,\mathbb{C}^2)\times\mathbb{C}$ with typical fiber C. Now the curvature forms (components) of these connections, namely $\Omega_0 = d\omega_0 - \omega_0\wedge\omega_1$, $\Omega_1 = d\omega_1 + 2\omega_0\wedge\omega_2$, and $\Omega_2 = d\omega_2 - \omega_1\wedge\omega_2$, have the property to lie in the closed ideal generated by $\{\omega^i\}_1^4$. This shows that our submodels $Z_i \subset Z$, described by (3.8a), are indeed to be associated with the vanishing of SL (2,C)-connections in $J^1(M,\mathbb{C}^2)\times\mathbb{C}$.

As for (3.10), we note that the Bäcklund maps are defined through two equations instead of one. However, they do present a nice feature in being linear in the fields. In particular, (3.10f) has a non-negligible importance. As its integrability conditions, by construction, yield Z_6, it therefore gives us that pair of linear systems which could serve as a basis for an inverse scattering transform type of problem, i.e., a Lax pair; in particular, it we set $g_2 = 0$, this pair is exactly the one which Kuznetsov and Mikhailov used when they investigated the classical massive Thirring model with the inverse scattering transform formalism.[11]

We thus realize that the prolongation method is quite rich in content. In addition, it can provide us with conservation laws which might not appear evident from a superficial examination of Z_i, as we shall soon see. Besides that, the Bäcklund transformations which they may furnish can also be very useful, in their turn, by inducing quite nontrivial solutions.

Let us come back to (3.8) and (3.9). We shall examine them case by case (i.e., a to f) and interest ourselves with (pseudo-) conservation laws which may possibly be obtained from them.

(a) Trivial case: arithmetic numbers are conserved.

(b) If $v = \alpha y$ then apply a transformation $y \to e^{\alpha y}$. Now, $[\partial_x, \partial_t]y = 0$ implies that $(|\psi_1|^2 + |\psi_2|^2)_{,t} + (|\psi_1|^2 - |\psi_2|^2)_{,x} = 0$. Hence we have a conserved density $\int_{\mathbb{R}}(|\psi_1|^2 + |\psi_2|^2)dx = \int_{\mathbb{R}} \Psi^\dagger\Psi\, dx$ and a conserved flow $\int_{\mathbb{R}}(|\psi_1|^2 - |\psi_2|^2)dt = \int_{\mathbb{R}} \Psi^\dagger\gamma^5\Psi\, dt$ (provided, naturally, that these integrals converge to some finite values).

(c) Here, the conserved density is $\int_{\mathbb{R}}(\psi_2^2 - \psi_1^2)dx = \int_{\mathbb{R}} \Psi^T\gamma^5\Psi\, dx$ and the conserved flow is $\int_{\mathbb{R}}(\psi_1^2 + \psi_2^2)dt = \int_{\mathbb{R}} \Psi^T\Psi\, dt$.

(d) In this case, the conserved quantities are those of (b) and (c).

(e) Here, we get pseudoconserved quantities (though "disguised" conserved quantities would be a more appropriate term). The pseudoconserved density and pseudoconserved flow are

$$\int_{\mathbb{R}} \{4ig_2\Psi^\dagger\Psi y - \Psi^T\gamma^5\Psi y^2 + 4g_2g_4\Psi^\dagger\gamma^5\Psi^*\}dx,$$

$$\int_{\mathbb{R}} \{\Psi^T\Psi y^2 - 4g_2g_4\Psi^\dagger\Psi^* - 4ig_2\Psi^\dagger\gamma^5\Psi y\}dt. \tag{3.11}$$

(f) Similarly, the pseudoconserved quantities are

$$\int_{\mathbb{R}} \{i[2g_1(|\psi_2|^2 - |\psi_1|^2) + 2g_2(|\psi_2|^2 + |\psi_1|^2) + m(\sigma - \sigma^{-1})]y + (\psi_1 - \sigma\psi_2)y^2 - 2mg_1(\bar\psi_2 - \sigma^{-1}\bar\psi_1)\}dx, \tag{3.12}$$

$$\int_{\mathbb{R}} \{-i[2g_1(|\psi_2|^2 + |\psi_1|^2) - 2g_2(|\psi_2|^2 - |\psi_1|^2) + m(\sigma + \sigma^{-1})]y + (\psi_1 + \sigma\psi_2)y^2 + 2mg_1(\bar\psi_2 + \sigma^{-1}\bar\psi_1)\}dt.$$

Naturally, (3.11) and (3.12) are not really true conserved quantities, according to the usual meaning. However, they do become so from the moment that the pseudopotentials "y's" are explicitly solved in terms of the fields. It is sometimes possible to generate true constants of the motion, in a local sense though, when the Bäcklund maps do involve a free parameter. This is so for the case (f), when $g_1 \neq 0$. To get those quantities, let us first modify the Bäcklund map by dividing (3.9f) by $\sqrt{2mg_1}\lambda^{-1}$, $\lambda^2 = \sigma$, and by applying a transformation $y \to i\sqrt{2mg_1}\lambda^{-1}y$. The Bäcklund map then can be written

$$y_{,\xi} = -i\sqrt{2mg_1}\lambda^{-1}\psi_1 y^2 - i[m\lambda^{-2} - 2(g_1 - g_2)|\psi_1|^2]y + i\sqrt{2mg_1}\lambda^{-1}\bar\psi_1, \tag{3.9f'}$$

$$y_{,\eta} = -i\sqrt{2mg_1}\lambda\psi_2 y^2 - i[m\lambda^2 - 2(g_1 + g_2)|\psi_2|^2]y + i\sqrt{2mg_1}\lambda\bar\psi_2.$$

Solving for y^2 and eliminating $|\psi_1|^2, |\psi_2|^2$ with the field equations, we get

$$i\lambda(\psi_2 y)_{,\xi} - i\lambda^{-1}(\psi_1 y)_{,\eta} = \sqrt{2mg_1}(\psi_1\bar\psi_2 - \bar\psi_1\psi_2). \tag{3.13}$$

Assume then that y is an analytic function of λ in some open set which contains $\lambda = 0$. This allows us, by definition, to expand y in a power series with respect to λ; in particular, we may choose this expansion to be

$$y = \sum_{k=0}^{\infty} y_k \lambda^{2k+1}. \tag{3.14}$$

We substitute this into (3.13) and get

$$i\sum_{k=0}^{\infty}\{\lambda^{2k+2}(\psi_2 y_k)_{,\xi}-\lambda^{2k}(\psi_1 y_k)_{,\eta}\}$$
$$=\sqrt{2mg_1}(\psi_1\bar{\psi}_2-\bar{\psi}_1\psi_2).$$

Observe that all the powers of λ are even ones. We thus obtain, for all k's,

$$(\psi_2 y_k)_{,\xi}-(\psi_1 y_{k+1})_{,\eta}=0, \tag{3.15}$$

and a defining relation for y_0,

$$-i(\psi_1 y_0)_{,\eta}=\sqrt{2mg_1}(\psi_1\bar{\psi}_2-\bar{\psi}_1\psi_2).$$

This yields the conservation laws

$$(\psi_2 y_k-\psi_1 y_{k+1})_{,t}+(\psi_2 y_k+\psi_1 y_{k+1})_{,x}=0;$$

therefore the following objects are conserved quantities:

$$C_k=\int_{\mathbf{R}}(\psi_2 y_k-\psi_1 y_{k+1})dx.$$

To obtain these, we begin by expanding (3.15) and by replacing $\psi_{2,\xi}$, $\psi_{1,\eta}$ in this with the help of the field equations. We then expand $iy_{,\eta}$ into a power series. The results are expressions for y_k in terms of the fields only:

$$\begin{aligned}
y_0&=m^{-1}\sqrt{2mg_1}\bar{\psi}_1,\\
y_1&=im^{-2}\sqrt{2mg_1}[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1,\\
y_2&=-m^{-3}\sqrt{2mg_1}[\partial_\xi+2i(g_1+g_2)|\psi_1|^2]\\
&\quad\times[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1,\\
y_3&=-im^{-4}\sqrt{2mg_1}[\partial_\xi+2i(g_1+g_2)|\psi_1|^2]^2\\
&\quad\times[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1,\\
&\vdots\\
y_k&=m^{-1}\Big[2(g_1-g_2)|\psi_1|^2 y_{k-1}+i(y_{k-1})_{,\xi}\\
&\quad-\sqrt{2mg_1}\sum_{j=0}^{k-1}y_j y_{k-j-1}\Big],\\
&\vdots.
\end{aligned} \tag{3.16}$$

From this, we immediately get the following local conserved densities:

$$\begin{aligned}
C_0&=\int_{\mathbf{R}}\{\bar{\psi}_1\psi_2-im^{-1}[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1\}dx,\\
C_1&=\int_{\mathbf{R}}\{i\psi_2[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1\\
&\quad+m^{-1}\psi_1[\partial_\xi+2i(g_1+g_2)|\psi_1|^2]\\
&\quad\times[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1\}dx,\\
C_2&=\int_{\mathbf{R}}\{\psi_2[\partial_\xi+2i(g_1+g_2)|\psi_1|^2]\\
&\quad\times[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1-im^{-1}\psi_1\\
&\quad\times[\partial_\xi+2i(g_1+g_2)|\psi_1|^2]^2[\partial_\xi+2ig_2|\psi_1|^2]\bar{\psi}_1\\
&\quad-2m^{-1}g_1\psi_1^2[(\partial_\xi+2ig_2|\psi_1|^2)\bar{\psi}_1]^2\}dx,\\
&\vdots\\
C_{k+1}&=\int_{\mathbf{R}}\Big\{2(g_1-g_2)|\psi_1|^2[\psi_2 y_k-\psi_1 y_{k+1}]\\
&\quad+i[\psi_2 y_{k,\xi}-\psi_1 y_{k+1,\xi}]\\
&\quad-\sqrt{2mg_1}\psi_1\Big[\sum_{j=0}^{k}y_j y_{k-j}\\
&\quad-\sum_{j=0}^{k-1}y_j y_{k-j-1}\Big]\Big\}dx,\\
&\vdots.
\end{aligned}$$

Remark: One can also suppose that y is an analytic function of λ^{-1} in some open set containing $\lambda^{-1}=0$. This will imply another infinite family of conserved densities which, this time, will be expressed in terms of ψ_2, $\bar{\psi}_2$, and derivatives of these with respect to η. A direct consequence of such families is the complete integrability of the subsytem Z_f.

IV. THE BÄCKLUND PROBLEM—OBTAINING BÄCKLUND TRANSFORMATIONS

A method for solving this problem has been suggested by Wahlquist and Estabrook in Ref. 8. We shall follow a similar path but use a differential formulation instead of a Pfaffian-like one. What we shall look for, actually, are mappings F: $\mathbb{C}^2\times\mathbb{C}\to\mathbb{C}^2$ with local representation $\tilde{\psi}_i=F_i(\psi_j,\bar{\psi}_j;y,\bar{y})$ such that $\tilde{\Psi}$ is a solution of Z_i whenever Ψ itself is one. Crudely put, the method is as follows. We first assume that $\tilde{\Psi}(\xi,\eta)$ does exist and require that it satisfy Z_i whenever $\Psi(\xi,\eta)$ does. We then substitute the $\tilde{\psi}_j,\tilde{\psi}_j$ into (3.9). Finally we demand that the differential system thus obtained for $F(\tilde{\Psi})$ be an identity in the old variables ψ_j, $\bar{\psi}_j$. This will give us a set of conditions which, if solvable, will yield a Bäcklund transformation. Let us recall the field equations:

$$\begin{aligned}
i\psi_{2,\xi}&=m\psi_1+b_0|\psi_1|^2\psi_2+c_0\psi_1^2\bar{\psi}_2,\\
i\psi_{1,\eta}&=m\psi_2+b_1|\psi_2|^2\psi_1+c_1\psi_2^2\bar{\psi}_1.
\end{aligned} \tag{4.1}$$

A $\tilde{\Psi}$ is also a solution, then

$$\begin{aligned}
i\tilde{\psi}_{2,\xi}&=m\tilde{\psi}_1+b_0|\tilde{\psi}_1|^2\tilde{\psi}_2+c_0\tilde{\psi}_1^2\bar{\tilde{\psi}}_2,\\
i\tilde{\psi}_{1,\eta}&=m\tilde{\psi}_2+b_1|\tilde{\psi}_2|^2\tilde{\psi}_1+c_1\tilde{\psi}_2^2\bar{\tilde{\psi}}_1.
\end{aligned} \tag{4.2}$$

For the sake of simplicity, we shall further assume that $\tilde{\Psi}$ is of the form

$$\begin{aligned}
\tilde{\psi}_1&=\pi(y,\bar{y})\psi_1+\tau(y,\bar{y}),\\
\tilde{\psi}_2&=p(y,\bar{y})\psi_2+q(y,\bar{y}).
\end{aligned}$$

Using this and (4.1), (4.2) becomes equivalent to this other pair:

$$\begin{aligned}
i\tilde{\psi}_{2,\xi}&=p(m\psi_1+b_0|\psi_1|^2\psi_2+c_0\psi_1^2\bar{\psi}_2)\\
&\quad+i\psi_2(y_{,\xi}p_{,y}+\bar{y}_{,\xi}p_{,\bar{y}})+i(y_{,\xi}q_{,y}+\bar{y}_{,\xi}q_{\bar{y}})\\
&=m(\pi\psi_1+\tau)+c_0[\bar{p}\pi^2\psi_1^2\bar{\psi}_2+2\bar{p}\pi\tau\psi_1\bar{\psi}_2\\
&\quad+\bar{p}\tau^2\bar{\psi}_2+\bar{q}\pi^2\psi_1^2+2\bar{q}\pi\tau\psi_1+\bar{q}\tau^2]\\
&\quad+b_0[p|\pi|^2\psi_1|^2\psi_2+p\pi\bar{\tau}\psi_1\psi_2+p\bar{\pi}\tau\bar{\psi}_1\psi_2\\
&\quad+p|\tau|^2\psi_2+q|\pi|^2|\psi_1|^2\\
&\quad+q\pi\bar{\tau}\psi_1+q\bar{\pi}\tau\bar{\psi}_1+q|\tau|^2],\\
i\tilde{\psi}_{1,\eta}&=\pi(m\psi_2+b_1|\psi_2|^2\psi_1+c_1\psi_2^2\bar{\psi}_1)\\
&\quad+i\psi_1(y_{,\eta}\pi_{,y}+\bar{y}_{,\eta}\pi_{\bar{y}})+i(y_{,\eta}\tau_{,y}+\bar{y}_{,\eta}\tau_{,\bar{y}})
\end{aligned} \tag{4.3}$$

$$= m(p\psi_2 + q) + c_1[p^2\bar{\pi}\bar{\psi}_1\psi_2^2 + 2pq\bar{\pi}\bar{\psi}_1\psi_2 + q^2\bar{\pi}\bar{\psi}_1 + p^2\bar{\tau}\psi_2^2 + 2pq\bar{\tau}\psi_2 + q^2\bar{\tau}] + b_1[|p|^2\pi\psi_1|\psi_2|^2 + p\bar{q}\pi\psi_1\psi_2 + \bar{p}q\pi\psi_1\bar{\psi}_2 + |q|^2\pi\psi_1 + |p|^2\tau|\psi_2|^2 + \bar{p}q\tau\bar{\psi}_2 + p\bar{q}\tau\psi_2 + |q|^2\tau].$$

In these expressions we replace the $y_{,\xi}$ and $y_{,\eta}$ from (3.8). For all subsystems, save Z_f with $g_1 \neq 0$, we are rapidly lead to the same trivial Bäcklund transformation: $\tilde{\Psi} = e^{i\theta}\Psi$, $\theta \in \mathbb{R}$; we do not learn anything new from this (we already knew this symmetry). For Z_f, however, things are different. Equations (4.3) transform into a system of 16 equations to be solved for p,q,π,τ, and their derivatives with respect to $y, \bar{y}$. It proves to be indeed solvable and we find a nontrivial Bäcklund transformation $B(\lambda): \mathbb{C}^2 \times \mathbb{C} \to \mathbb{C}^2: \Psi \mapsto \tilde{\Psi}$, which can be explicitly written as ($\lambda^2 = \sigma$)

$$\tilde{\psi}_1 = C\left[\frac{\lambda + \bar{\lambda}|y|^2}{\bar{\lambda} + \lambda|y|^2}\right]^{g_2/g_1} \times \left[\frac{\bar{\lambda}^{-1} + \lambda^{-1}|y|^2}{\lambda^{-1} + \bar{\lambda}^{-1}|y|^2}\psi_1 + \frac{m(\lambda^{-2} - \bar{\lambda}^{-2})\bar{y}}{\sqrt{2mg_1}(\lambda^{-1} + \bar{\lambda}^{-1}|y|^2)}\right],$$
$$\tilde{\psi}_2 = C\left[\frac{\lambda + \bar{\lambda}|y|^2}{\bar{\lambda} + \lambda|y|^2}\right]^{g_2/g_1} \times \left[\frac{\bar{\lambda} + \lambda|y|^2}{\lambda + \bar{\lambda}|y|^2}\psi_2 + \frac{m(\lambda^2 - \bar{\lambda}^2)\bar{y}}{\sqrt{2mg_1}(\lambda + \bar{\lambda}|y|^2)}\right], \tag{4.4}$$

where $|C|^2 = 1$. One may verify that $\tilde{\Psi}$ is indeed a solution simply by substituting (4.4) in the field equations (3.8f). As a special case, notice that if we set $g_2 = 0$, then (4.4) reduces to the usual Bäcklund transformation for the classical massive Thirring model as mentioned, for instance, in Ref. 6 (up to a misprint of $\bar{y}$ as y).

In this procedure that we just completed, we required $\tilde{\Psi}$ to be linear in Ψ. We could have done otherwise and demanded that it would rather be linear in Ψ^*. As a matter of fact, the relationship between $\tilde{\Psi}$ and Ψ^* is quite nice. To obtain it, recall (3.9f′) and its complex conjugate that we multiply by $\bar{y}, y$, respectively. Eliminating $|\psi_i|^2$, we get

$$|y|^2_{,\eta} = i\sqrt{2mg_1}[(\lambda + \bar{\lambda}|y|^2)\bar{y}\bar{\psi}_2 - (\bar{\lambda} + \lambda|y|^2)y\psi_2] - im(\lambda^2 - \bar{\lambda}^2)|y|^2,$$
$$|y|^2_{,\xi} = i\sqrt{2mg_1}[(\lambda^{-1} + \bar{\lambda}^{-1}|y|^2)\bar{y}\bar{\psi}_1 - (\bar{\lambda}^{-1} + \lambda^{-1}|y|^2)y\psi_1] - im(\lambda^{-2} - \bar{\lambda}^{-2})|y|^2.$$

In this we replace ψ_1, ψ_2 as we obtain them by inverting the Bäcklund transformation (4.4). This yields quite simple identities:

$$|y|^2_{,\eta} = i\sqrt{2mg_1}(\lambda + \bar{\lambda}|y|^2) \times \left\{\bar{y}\bar{\psi}_2 - C^{-1}\left[\frac{\bar{\lambda} + \lambda|y|^2}{\lambda + \bar{\lambda}|y|^2}\right]^{g_2/g_1} y\tilde{\psi}_2\right\},$$
$$|y|^2_{,\xi} = i\sqrt{2mg_1}(\lambda^{-1} + \bar{\lambda}^{-1}|y|^2) \times \left\{\bar{y}\bar{\psi}_1 - C^{-1}\left[\frac{\bar{\lambda} + \lambda|y|^2}{\lambda + \bar{\lambda}|y|^2}\right]^{g_2/g_1} y\tilde{\psi}_1\right\}.$$

For the classical massive Thirring model ($g_2 = 0$), with $C = 1$, these identities do assume a very compact form:

$$|y|^2_{,\eta} = i\sqrt{2mg_1}(\lambda + \bar{\lambda}|y|^2)(\bar{y}\bar{\psi}_2 - y\tilde{\psi}_2),$$
$$|y|^2_{,\xi} = i\sqrt{2mg_1}(\lambda^{-1} + \bar{\lambda}^{-1}|y|^2)(\bar{y}\bar{\psi}_1 - y\tilde{\psi}_1).$$

These identities could be useful, amongst other things, for establishing recurrence formulas in view of obtaining chains of solutions.

V. SOLUTIONS OF THE MODEL

Naturally, the very next thing one would like to do is to see what kind of solutions this transformation gives rise to. Let us consider the trivial solution $\Psi = 0$. In this case, (4.4) simply becomes

$$\tilde{\psi}_1 = \frac{-(\lambda + \bar{\lambda}|y|^2)}{(\bar{\lambda} + \lambda|y|^2)|\lambda|^2}\tilde{\psi}_2,$$
$$\tilde{\psi}_2 = C\left[\frac{\lambda + \bar{\lambda}|y|^2}{\bar{\lambda} + \lambda|y|^2}\right]^{g_2/g_1} \frac{m(\lambda^2 - \bar{\lambda}^2)\bar{y}}{\sqrt{2mg_1}(\lambda + \bar{\lambda}|y|^2)}.$$

and the Bäcklund map (3.9f′) gets reduced to

$$iy_{,\xi} = m\lambda^{-2}y, \quad iy_{,\eta} = m\lambda^2 y.$$

Up to a multiplicative complex factor, the solution to this is

$$y = \exp(-im(\lambda^{-2}\xi + \lambda^2\eta)),$$

with

$$|y|^2 = \exp(im(\lambda^2 - \bar{\lambda}^2)(\xi - |\lambda|^4\eta)/|\lambda|^4).$$

We want to decompose $\tilde{\Psi}$ into its real and imaginary parts. In order to do that, we set $\lambda = \mu + i\nu$. After many tedious calculations, we find that

$$\mathrm{Re}(\tilde{\psi}_2) = \frac{2m\mu\nu[-\mu\sin\beta\cosh\omega + \nu\cos\beta\sinh\omega]}{\sqrt{2mg_1}(\mu^2\cosh^2\omega + \nu^2\sinh^2\omega)},$$
$$\mathrm{Im}(\tilde{\psi}_2) = \frac{2m\mu\nu[\mu\cos\beta\cosh\omega + \nu\sin\beta\sinh\omega]}{\sqrt{2mg_1}(\mu^2\cosh^2\omega + \nu^2\sinh^2\omega)}, \tag{5.1}$$
$$|\tilde{\psi}_2|^2 = \frac{2m\mu^2\nu^2/g_1}{\mu^2\cosh^2\omega + \nu^2\sinh^2\omega},$$
$$\mathrm{Re}(\tilde{\psi}_1) = \frac{2m\mu\nu[\mu\sin\beta\cosh\omega + \nu\cos\beta\sinh\omega]}{(\mu^2 + \nu^2)\sqrt{2mg_1}(\mu^2\cosh^2\omega + \nu^2\sinh^2\omega)},$$
$$\mathrm{Im}(\tilde{\psi}_1) = \frac{2m\mu\nu[-\mu\cos\beta\cosh\omega + \nu\sin\beta\sinh\omega]}{(\mu^2 + \nu^2)\sqrt{2mg_1}(\mu^2\cosh^2\omega + \nu^2\sinh^2\omega)}, \tag{5.2}$$
$$|\tilde{\psi}_1|^2 = |\tilde{\psi}_2|^2/(\mu^2 + \nu^2)^2,$$

where

$$\beta = \alpha + \theta, \quad C = e^{i\alpha},$$
$$\omega = -2m\mu\nu[\xi - (\mu^2 + \nu^2)\eta]/(\mu^2 + \nu^2)^2,$$
$$\theta = \frac{m(\mu^2 - \nu^2)}{(\mu^2 + \nu^2)^2}[\xi + (\mu^2 + \nu^2)\eta] + \left(\frac{g_2}{g_1}\right)\tan^{-1}\left[\frac{2(\nu/\mu)\tanh\omega}{1 - (\nu/\mu)^2\tanh^2\omega}\right].$$

In order to best visualize the form and the evolution of these quantities, let us set

$$m = \tfrac{1}{2}, \quad g_1 = 1, \quad g_2 = 2,$$
$$C = 1 \quad (\text{i.e., } \alpha = 0), \quad \lambda = 1 + 2i.$$

Figure 1 illustrates the behavior of $\mathrm{Re}(\tilde{\psi}_1)$, $\mathrm{Im}(\tilde{\psi}_1)$, and $|\tilde{\psi}_1|$

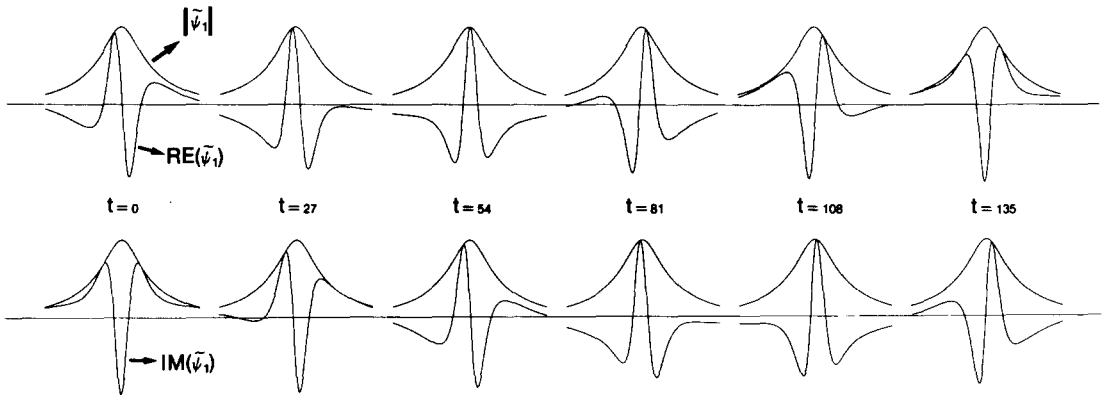

FIG. 1. The behaviors of $\mathrm{Re}(\tilde{\Psi}_2)$, $\mathrm{Im}(\tilde{\psi}_2)$, and $|\tilde{\psi}_2|$ for a few distinct values of time.

for a few distinct values of time [$\mathrm{Re}(\tilde{\psi}_2)$, $\mathrm{Im}(\tilde{\psi}_2)$, and $|\tilde{\psi}_2|$ behave in an analogous manner].

Again, one may verify that (5.1) and (5.2) do indeed constitute a solution merely by placing them into (3.8f). Let us now make a few remarks on this solution. First, we notice that $|\tilde{\psi}_i|^2$ is a function of the single quantity ω and thus is a nondispersive traveling wave, localized, with a constant velocity given by

$$v = \frac{(\mu^2 + \nu^2) - 1}{(\mu^2 + \nu^2) + 1} = \frac{r^2 - 1}{r^2 + 1} = \tanh[\ln(r)] = v(r).$$

Now, as $\lambda \in \mathbb{C} \setminus \{0\}$, then $r \in [0, \infty)$; therefore $|\tilde{\psi}_i|^2$ is to be considered as an "infraluminic" object, for v: $[0, \infty) \mapsto (-1, 1)$ (i.e., the limit speed is "1" natural units). If λ stands on the unit circle, then $r = 1$ and $v = 0$: therefore the lump-shaped $|\tilde{\psi}_i|^2$'s remain still! If it is inside or outside of the unit circle, then they have negative or positive velocities, respectively (for our numerical example, $v = 2/3$ in natural units). Moreover, note that $v(1/r) = -v(r)$. It is also possible to define a quantity which could be interpreted as a measure of the (finite) energy of the solution, namely,

$$E = \frac{m}{\sqrt{1 - v^2}} = \frac{m(r^2 + 1)}{2r} = E(r).$$

If we now look at the fields themselves (the components of $\tilde{\Psi}$), we first notice that they are bounded, in absolute value, by their norms (the lumps). We then remark that they are sorts of oscillating functions. This is a characteristic behavior which is reminiscent of the soliton solutions of the cubic nonlinear Schrödinger equation. Still there is an important difference. For the Schrödinger equation, the solitons are oscillating with a fixed frequency since they are of the form

$$\phi = a\sqrt{2\lambda/\nu}\,\mathrm{sech}[a(x - 2bt)]\exp[ibx + i\lambda(a^2 - b^2)t]$$

(for $\lambda\phi_{,xx} + i\phi_{,t} = \nu|\phi|^2$, with $\lambda\nu < 0$), whereas our solutions for the extended Thirring system are not oscillating at such a fixed frequency. The reason for this lies within the form of θ which involves a peculiar dependence on ω. However, for the classical massive Thirring system, this dependence vanishes and the solutions are thus much more like those of the nonlinear Schrödinger equation. It may be worth mentioning that this peculiar oscillating behavior reminds us of that of the so-called "boomerons" introduced by Calogero and Degasperis.[12]

A pertinent question that we may now ask ourselves is whether or not the solution which we obtained should be termed solitons. A first remark it that according to the dedicated definition they should not even be called solitary waves. Yet, it remains that they are localized and nondispersive, in a certain sense, functions. However, to label them as solitons is a bit problematic. Indeed, before doing so, one should formally look at, and analyze, their interaction with other objects of a similar kind. Put in other words, this means that one should explicitly construct two-lump (or "multilump") solutions. At present, it has been impossible to do so. Actually, the tools which we gave ourselves here prove to be inefficient for such a construction. First of all, it it obvious that the Bäcklund map (3.9f') cannot be used for deriving a superposition rule since the pseudopotential y is one-dimensional whereas Ψ has two components. Moreover, it appears that it would be rather difficult, if it is at all possible, to verify if the Bäcklund transformation commutes with respect to an interchange of parameter values, i.e., if $B(\lambda) \circ B(\mu) = B(\mu) \circ B(\lambda)$. In the same spirit, the two-dimensional Bäcklund map (3.10f) does not seem to yield a Bäcklund transformation other than the trivial one. As an alternative way out, one could consider a repetitive utilization of the Bäcklund transformation (4.4). We performed a first step by applying it to the solution $\Psi = 0$; the second step would consist in feeding (5.1) and (5.2) back into (4.4) and (3.9f'), and then to solve this latter system. It is immediately evident that this is a most difficult vector Riccati system. Finally, a third way out would be to make use of the inverse scattering transform formalism, since we already have the necessary basic linear equations (or Lax pair) which are needed for that purpose, namely (3.10f). Technically speaking, this should appear to be a viable way. Actually, comparing our Lax pair to the one used by Kuznetsov and Mikhailov,[11] one should discover that the direct scattering problem is exactly the same as theirs (up to a redefinition of parameters) and therefore the quasitotality of the formalism remains unchanged; the only minor difference is contained in the fact that the scattering data will evolve according to a slightly different equation. An additional argument which also tells us to push along this line is the following fact. Using the symmetry reduction technique described in Ref. 13, one can obtain ordinary differential equations which are exact reductions of the system Z_6 given by (3.8f) and to show that these have no movable critical points [i.e., movable singularities other than poles (of any order)], hence to show that they have the Pain-

levé property. This property can also be established in a more direct manner from (3.8f) without any reductions by using the technique recently proposed by Weiss.[14] According to the Painlevé conjecture,[15] this property is a necessary condition for the solvability of (3.8f) by an inverse scattering transform.

VI. CONCLUSION

We introduced a nonlinear system which contains the classical massive Thirring model as a special case and preserves relativistic invariance; in fact, this system is invariant under a Lie point group $P(1,1)\times U(1)$. Having constructed a prolongation structure associated with this differential system by using the method of Wahlquist and Estabrook, we succeeded in breaking the system into a family of subsystems classified with respect to the different types of allowed Bäcklund maps. Among these, one stands out of the ranks and prove to be quite interesting; it is the restriction of (2.1) to the current-pseudocurrent case (i.e., $g_3 = g_4 = 0$, $g_1 \neq 0$), a sort of natural extension of the Thirring model. Actually, one can show that, in a certain sense, it is gauge equivalent to the Thirring model.[16] In this particular extension appears a free parameter (σ or λ) which is very important. It was mentioned that it takes its origin as a symmetry of the prolongation structure; to be more precise, it is indicative of a Kac–Moody symmetry algebra connected with the Zakharov–Shabat (or Lax) pair (3.10f). Because of this parameter, we were able to generate an infinite family of local conservation laws, thus establishing the complete integrability of the corresponding subsystem. We also deduced, from the Bäcklund map, the Lax pair of linear equations which is the basis of an associated inverse scattering problem. Finally, we constructed a nontrivial Bäcklund trnsformation which we used in order to show that the subsystem does admit some sort of solitons as possible solutions. One-soliton solutions were explicitly computed.

Let us end by mentioning a few points which merit a deeper investigation. First, we must point out that the prolongation method, though it is very nice from the practical point of view, may not yield the most general Bäcklund map. For this particular purpose, one should ultimately prefer the method devised by Clairin,[17] or even follow a procedure recently proposed by Denes and Finley.[18] Along the same lines, for this model, as well as many other two-dimensional completely integrable ones, Bäcklund transformations are not exactly the right kind of objects to look for, especially if we have in mind to construct soliton solutions. Rather, one should try to build so-called multi-Bäcklund transformations. This is the object of Ref. 16 in which multisoliton solutions will be explicitly constructed for the Thirring system and other systems which are gauge equivalent to it, using the Zakharov–Mikhailov–Shabat dressing method.

ACKNOWLEDGMENTS

The author wishes to express his gratitude to P. Winternitz for many helpful discussions.

The author also wishes to thank the Fonds FCAC and NSERC for their support.

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Landau–Lifshitz and higher-order nonlinear systems gauge generated from nonlinear Schrödinger type equations

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(Received 29 December 1983; accepted for publication 2 March 1984)

New Landau–Lifshitz (LL) and higher-order nonlinear systems gauge generated from nonlinear Schrödinger (NS) type equations are presented. The consequences of gauge equivalence between different dynamical systems are discussed. The gauge connections among various LL and NS equations are found and depicted through a schematic representation.

PACS numbers: 02.30.Jr, 11.15. − q, 11.10.Lm, 02.20. + b

I. INTRODUCTION

In recent years growing interest has been focused on the discovery of gauge connection between various nonlinear systems.[1–9] Such interconnections allow us not only to systematize and group together the large number of nonlinear systems already known, but also to conclude about the properties of a system knowing the corresponding properties of its gauge-equivalent counterpart. One of such gauge-connected systems which deserves much physical interest is the Landau–Lifshitz equation (LLE) and the nonlinear Schrödinger equation (NSE).[1,2] Recently, the above equivalence between LLE and NSE has been generalized for higher unitary groups,[3] for Grassmannian manifolds,[6] and for noncompact groups,[7,8] and has been extended also to unconstraint SU(N) models.[9] Besides the standard NSE, however, different other types of integrable NSE systems are known in literature.[10–14] Our aim is to find different generalized Landau–Lifshitz equations which are gauge equivalent to them. New higher-order nonlinear systems are also obtained through U(1)-gauge transformations of NS type equations. Since the proposed nonlinear equations being gauge equivalent to integrable NS systems are also integrable, they might be useful in approximating quasi-one-dimensional real models.

The paper is organized as follows. In Sec. II, the consequences of the gauge equivalence between different systems are discussed. In Sec. III we deduce new Landau–Lifshitz type systems. Higher-order nonlinear equations are found in Sec. IV. Using the gauge freedom of LLE relative to subgroup $H \subset G$ it has been shown in Sec. V that all H-transformed NSE are also gauge equivalent to a given LLE. This section also presents a schematic diagram showing the gauge connection between all the different systems proposed. Sec. VI is the concluding section.

II. GAUGE EQUIVALENCE OF NONLINEAR EVOLUTIONARY SYSTEMS

We discuss in brief the Lax pair formalism of nonlinear evolutionary systems and how to construct their gauge-equivalent counterparts. We have the given evolution equation $\hat{L}q = 0$ with $\hat{L}$ being a nonlinear differential operator acting on field q. The linear problem associated with the given system may be expressed as

$$dv = \Omega v\,, \tag{2.1a}$$

where d denotes exterior differentiation, Ω is a 1-form matrix valued on the Lie algebra of some matrix group G, and v is the matrix 0-form. In (1 + 1) space-time, Eq. (2.1a) in the component form looks as

$$\Phi_x = U\Phi\,, \quad \Phi_t = V\Phi\,, \tag{2.1b}$$

where the Jost function Φ and U and V are complex matrix functions of the field q, its derivatives, independent variables x and t, and the spectral parameter λ. The integrability of (2.1a), which is equivalent to the flatness condition, requires that the following two-form Θ should vanish:

$$\Theta = d\Omega - \Omega \wedge \Omega = 0\,, \tag{2.2a}$$

where $\wedge$ denotes exterior product. In component form the compatibility condition $\Phi_{xt} = \Phi_{tx}$, which is equivalent to (2.2a), is given by

$$U_t - V_x + [U,V] = 0\,. \tag{2.2b}$$

Here, U and V operators are so constructed that the original nonlinear evolution equation is represented by (2.2b), which may also be expressed in the Lax form

$$L_t = [A,L]\,, \tag{2.3}$$

with $L\Phi = \lambda\Phi$ and $\Phi_t = A\Phi$.

Now for real λ, $\Phi \in G$, G being a compact or noncompact Lie group, and under the local gauge transformation relative to the group element

$$g(x,t;\lambda_0) = \Phi(x,t;\lambda)|_{\lambda=\lambda_c} \in G\,, \tag{2.4}$$

the Jost function changes as

$$\Phi \to \Psi(x,t;\lambda,\lambda_0) = g^{-1}(x,t;\lambda_0)\Phi(x,t;\lambda)\,, \tag{2.5}$$

and the corresponding linear system associated with the new Jost function can be given by

$$\Psi_x = U'\Psi\,, \quad \Psi_t = V'\Psi\,, \tag{2.6}$$

with

$$\begin{aligned} U' &= g^{-1}Ug - g^{-1}g_x = g^{-1}(U - U_0)g\,, \\ V' &= g^{-1}Vg - g^{-1}g_t = g^{-1}(V - V_0)g\,, \end{aligned} \tag{2.7}$$

since

$$g_x g^{-1} = U_0 = U|_{\lambda=\lambda_0} \quad \text{and} \quad g_t g^{-1} = V_0 = V|_{\lambda=\lambda_0}\,. \tag{2.8}$$

The compatibility condition of (2.6) gives now the new gauge-equivalent equation

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$$U_t' - V_x' + [U',V'] = g^{-1}\{(U_t - V_x + [U,V]) - (U_{0t} - V_{0x} + [U_0,V_0])\}g = 0, \quad (2.9)$$

relative to a new field S: $\hat{L}'S = 0$, $\hat{L}'$ being some nonlinear operator acting on S. Note that gauge transformations like (2.4), but depending on the spectral parameter λ, may also construct Backlund transformation[15] generating new solutions from the given one, for the same evolution equation. We are however interested only in those gauge transformations (depending on λ_0 but not on λ) which yield new nonlinear equations different from the given one.

If all the properties of the initial model are known to us, it is interesting to ask whether it is also possible to find the corresponding properties of its gauge-equivalent counterparts. We find that the answer is affirmative in most of the cases. Let the scattering matrix T of the initial system be given by

$$\Phi_- = \Phi_+ T,$$

where Φ_+, Φ_- are known Jost functions with their asymptotics given at $\pm\infty$, respectively. Then it is not hard to get that the scattering matrix of its gauge-equivalent system should be given by

$$T' = \Psi_+^{-1}\Psi_- = \Phi_+^{-1} g_+ g_-^{-1} \Phi_- = (\Phi_+^{-1} g_+ T_0^{-1} g_+^{-1} \Phi_+) T,$$

$$\text{with} \quad T_0 = T(\lambda = \lambda_0). \quad (2.10)$$

Hence, knowing T and Φ_+ one can easily calculate T' and Ψ_+ which, in principle, should give all main properties of a system. Thus, knowing the soliton solutions of the initial system, one may deduce such solutions for its gauge-equivalent counterparts and the complete integrability property should also be common for all the gauge-connected systems. If, for example, we suppose NSE to be the initial system about which everything is known, then using (2.10) it is possible to evaluate the properties and solutions of its gauge-equivalent LLE without investigating the latter system individually. The field function S of LLE type equations may be expressed through the Jost function of NSE at $\lambda = \lambda_0$ (2.4) with $G = \mathrm{SU}(2)$ as

$$S = g^{-1}\sigma_3 g, \quad (2.11)$$

which due to (2.8) gives immediately

$$S_x = g^{-1}[\sigma_3, U_0]g \quad \text{and} \quad S_t = g^{-1}[\sigma_3, V_0]g. \quad (2.12)$$

As we will see below, relations (2.11) and (2.12) are very important for constructing explicitly various LLE systems. All the new models we discuss here are gauge equivalent to different NSE which are already well investigated. From relation (2.10), one gets also the somewhat unexpected result that the "pure soliton" states in one system (i.e., with reflectionless potential, $b = 0$) may not always give a pure soliton state (i.e., $b \neq 0$) in the gauge-transformed system. We like to stress here that usually λ_0 is taken to be trivial.[2] But, in general, $\lambda_0 = 0$ and it must be chosen from the continuum spectrum of the Jost function such that $g(x,t;\lambda_0)$ should have fixed group properties for all x and t.

III. GENERALIZED LLE TYPE EQUATIONS

Using the general method sketched out in Sec. II, we find different LLE from NS type equations.

A. Gauge-equivalent LLE and NSE

Gauge equivalence between standard NSE of the "attractive" type and the LLE with the associated $G = \mathrm{SU}(2)$ group has been established.[1,2] Analysis of the property of the Lie algebra corresponding to group G to which the Lax operators U,V belong, allows us to extend the above equivalence in the following way.[8] The attractive and repulsive type NSE

$$iq_t + q_{xx} \pm \beta |q|^2 q = 0, \quad \beta > 0, \quad (3.1)$$

are gauge equivalent to LLE,

$$S_t = (i/2)[S, S_{xx}] - 4\sqrt{2\beta}\,\lambda_0 S_x, \quad (3.2)$$

with $S \in \mathrm{SU}(2)/\mathrm{U}(1)$ and $S \in \mathrm{SU}(1,1)/\mathrm{U}(1)$, respectively. Here λ_0 may be chosen to be trivial for an "attractive" type equation with vanishing boundary condition $\lim_{x\to\pm\infty}|q| = 0$. For a nontrivial boundary condition, $\lim_{x\to\pm\infty}|q| = \mu \neq 0$, corresponding to the "repulsive" case, however, $|\lambda_0| > \mu$ due to the appearance of a gap in the continuum spectrum of λ (see Refs. 7 and 8). Note that the term proportional to λ_0 in (3.2) may be removed by the Galilean transformation $(x',t') = (x - 4\sqrt{2\beta}\,\lambda_0 t, t)$, i.e., with respect to a reference frame moving with a velocity $v_r = -4\sqrt{2\beta}\,\lambda_0$ relative to the original system. It is therefore clear that the soliton velocities of NSE and standard LLE may coincide only for vanishing boundary problems when λ_0 may be trivial, but they differ for nontrivial boundary conditions when $\lambda_0 \neq 0$. In what follows, similar to (3.1) and (3.2), the " + " and " − " signs in NS type equations will always correspond to LLE with compact, i.e., $S \in \mathrm{SU}(2)/\mathrm{U}(1)$, and noncompact, i.e., $S \in \mathrm{SU}(1,1)/\mathrm{U}(1)$, manifolds.

B. DLL gauge generated from DNS

The derivative nonlinear Schrödinger equation (DNS)[10]

$$q_t + q_{xx} \pm i\alpha(|q|^2 q)_x = 0, \quad \alpha > 0, \quad (3.3)$$

may be given by the linear system (2.1) with

$$U = -i\alpha\lambda^2\sigma_3 + \alpha\lambda A,$$

$$V = (-2i\alpha^2\lambda^4 \pm i\alpha^2|q|^2\lambda^2)\sigma_3 + 2\alpha^2\lambda^3 A + \alpha\lambda B, \quad (3.4)$$

where

$$A = \begin{pmatrix} 0, & q \\ \mp q^*, & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0, & iq_x \mp \alpha|q|^2 q \\ \pm iq_x^* + \alpha|q|^2 q^*, & 0 \end{pmatrix}. \quad (3.5)$$

Under the gauge transformation (2.5) the linear system (3.4) changes to the form (2.7) given by

$$U' = -i\alpha(\lambda^2 - \lambda_0^2)g^{-1}\sigma_3 g + \alpha(\lambda - \lambda_0)g^{-1}Ag,$$

and

$$V' = -2i\lambda^2\alpha^2(\lambda^4 - \lambda_0^4)g^{-1}\sigma_3 g + 2\alpha^2(\lambda^3 - \lambda_0^3)g^{-1}Ag - i\alpha^2(\lambda^2 - \lambda_0^2)g^{-1}\sigma_3 A^2 g + \alpha(\lambda - \lambda_0)g^{-1}Bg. \quad (3.6)$$

Using now (2.11) and (2.12) for explicit values (3.4), one gets with no difficulty the relation

$$S_x = 2\lambda_0 g^{-1}[\sigma_3, A]g = 2\lambda_0\alpha g^{-1}\sigma_3 A g, \quad (3.7a)$$

$$SS_x = 2\lambda_0 \alpha g^{-1} A g\,, \tag{3.7b}$$

$$-SS_x^2 = 4\lambda_0^2 \alpha^2 g^{-1}\sigma_3 A^2 g\,, \tag{3.7c}$$

and

$$S_t = 2\alpha^2\lambda_0^3 g^{-1}[\sigma_3, A]g + \alpha\lambda_0 g^{-1}[\sigma_3, B]g$$
$$= 2\alpha\lambda_0^2 S_x + 2\alpha\lambda_0 g^{-1}\sigma_3 B g\,. \tag{3.7d}$$

Hence,

$$S(S_t - 2\alpha\lambda_0^2 S_x) = 2\alpha\lambda_0 g^{-1} B g\,. \tag{3.7e}$$

Putting relations (3.7) in (3.6), we get finally

$$U' = -i\alpha(\lambda^2 - \lambda_0^2)S + (1/2\lambda_0)(\lambda - \lambda_0)SS_x\,,$$
$$V' = 2i\alpha^2(\lambda^4 - \lambda_0^4)S + (\alpha/\lambda_0)(\lambda^3 - \lambda_0^3)SS_x$$
$$+ i\frac{\lambda^2 - \lambda_0^2}{4\lambda_0^2} SS_x^2 + \frac{\lambda - \lambda_0}{2\lambda_0}(SS_t - 2\alpha\lambda_0^2 SS_x)\,. \tag{3.8}$$

The compatibility condition of (3.8) yields the LLE type system named the derivative Landau–Lifshitz (DLL) equation for definiteness:

$$S_t + \frac{1}{2i}[S, S_{xx}] - 4\alpha\lambda_0^2 S_x + \frac{1}{4\alpha\lambda_0^2} S_x^3 = 0\,, \quad \alpha > 0\,, \tag{3.9}$$

with $S \in \mathrm{SU(2)/U(1)}$ [SU(1,1)/U(t)] corresponding to $+(-)$ signs in (3.3).

C. MLL gauge generated from MNS

The mixed nonlinear Schrödinger equation (MNS), which is a hybrid of DNS and NSE, is given by[11]

$$iq_t + q_{xx} \pm \beta|q|^2 q \pm i\alpha(|q|^2 q)_x = 0\,, \quad \alpha > 0\,, \quad \beta > 0\,. \tag{3.10}$$

The corresponding linear system (2.1b) has

$$U = i(-\alpha\lambda^2 + \sqrt{2\beta}\,\lambda)\sigma_3 + (\alpha\lambda - \sqrt{\beta/2})A$$
$$V = \Big[-2i\alpha^2\lambda^4 + 4i\alpha\sqrt{2\beta}\,\lambda^3 + (-4i\beta \pm i\alpha^2|q|^2)\lambda^2$$
$$\mp i\alpha\sqrt{2\beta}\,\lambda|q|^2 \pm \frac{i}{2}\beta|q|^2\Big]\sigma_3$$
$$+ (2\alpha^2\lambda^3 - 3\sqrt{2\beta}\,\alpha\lambda^2 + 2\beta\lambda)A + (\alpha A - \sqrt{\beta/2})B\,, \tag{3.11}$$

where operators A and B are given by (3.5). Similar to the previous procedure we find the gauge equivalence of this system. The gauge-transformed operators are

$$U' = g^{-1}\{\delta\sigma_3 + aA\}g\,,$$
$$V' = g^{-1}\{\kappa\sigma_3 + bA + aB + \gamma\sigma_3 A^2\}g\,, \tag{3.12}$$

where

$$\delta = -i\alpha(\lambda^2 - \lambda_0^2) + i\sqrt{2\beta}\,(\lambda - \lambda_0)\,,$$
$$a = \alpha(\lambda - \lambda_0)\,,$$
$$\kappa = -2i\alpha^2(\lambda^4 - \lambda_0^4) + 4i\alpha\sqrt{2\beta}\,(\lambda^3 - \lambda_0^3)$$
$$- 4i\beta(\lambda^2 - \lambda_0^2)\,, \tag{3.13}$$
$$\sigma = +2\alpha^2(\lambda^3 - \lambda_0^3) - 3\alpha\sqrt{2\beta}\,(\lambda^2 - \lambda_0^2)$$
$$+ 2\beta(\lambda - \lambda_0)\,,$$
$$\gamma = -i\alpha^2(\lambda^2 - \lambda_0^2) + i\alpha\sqrt{2\beta}\,(\lambda - \lambda_0)\,.$$

From (2.11), (2.12) for (3.11) one gets

$$S_x = (c/2)g^{-1}[\sigma_3, A]g = cg^{-1}\sigma_3 A g\,, \tag{3.14a}$$

$$SS_x = cg^{-1}Ag\,, \tag{3.14b}$$

$$-SS_x^2 = c^2 g^{-1}\sigma_3 A^2 g\,, \tag{3.14c}$$

$$S_t = 2(\tilde{b}/c)S_x + cg^{-1}\sigma_3 B g\,, \tag{3.14d}$$

hence

$$S(S_t - 2(\tilde{b}/c)S_x) = cg^{-1}Bg\,, \tag{3.14e}$$

where

$$c = 2\alpha\lambda_0 - \sqrt{2\beta}\,,$$

and

$$\tilde{b} = -b(\lambda = 0) = 2\alpha^2\lambda_0^3 - 3\alpha\sqrt{2\beta}\,\lambda_0^2 + 2\beta\lambda_0\,. \tag{3.15}$$

Using relations (3.14) from (3.12) we easily obtain

$$U' = \delta S + (a/c)SS_x\,, \tag{3.16}$$

$$V' = \kappa S + \frac{b}{c}SS_x - \frac{\gamma}{c^2}SS_x^2 + \frac{a}{c}\left(SS_t - 2\frac{\tilde{b}}{c}SS_x\right), \tag{3.17}$$

which gives ultimately the gauge-equivalent generalized LLE [we call it the mixed Landau–Lifshitz (MLL) equation]

$$S_t + (\epsilon/2i)[S, S_{xx}] + (\gamma S_x + \rho S_x^3)$$
$$+ id\left\{[S_t, S_x] + \frac{1}{i}[SS_x, S_{xx}]\right\} = 0\,, \tag{3.18}$$

where

$$\epsilon = B/A\,, \quad \gamma = C/A\,, \quad \rho = D/A\,,$$
$$d = E/A\,, \quad e = F/A\,, \tag{3.19}$$

with

$$A = (\alpha^2\lambda_0^2 - 2\alpha\lambda_0\sqrt{2\beta}\,)/(c/2) + \sqrt{2\beta}\,,$$
$$B = 2\{(-\beta - 3\alpha^2\lambda_0^2)\sqrt{2\beta}\, + 2\alpha^3\lambda_0^3\}/c^2\,,$$
$$C = 2\{\sqrt{2\beta}\,(2\alpha^2\lambda_0^3 - 2\sqrt{2\beta}\,\lambda_0(\sqrt{2\beta}\, - 2\alpha\lambda_0))$$
$$- 2\alpha^3\lambda_0^4 + (2\tilde{b}/c)(2\alpha\lambda_0\sqrt{2\beta}\, - \alpha^2\lambda_0^2)\}/c\,, \tag{3.20}$$
$$D = -\alpha(\sqrt{2\beta}\, - \alpha\lambda_0)/c^2\,,$$
$$E = F = \alpha\sqrt{2\beta}\,/c^2\,.$$

In (3.18) the case $S \in \mathrm{SU(2)/U(1)}$ [SU(1,1)/U(1)] corresponds to the $+(-)$ type of Eq. (3.10). From (3.14) one can find also the generalization of the energy and current density relations between the LLE and NSE systems in the form

$$\mathrm{tr}(S^2{}_x) = \pm 2c^2|q|^2\,, \tag{3.21a}$$

and

$$\mathrm{tr}(S_x S_t) = c^2\{\mp i(qq_x^* - q^* q_x)$$
$$\pm 4(\tilde{b}/c)|q|^2 - 2\alpha|q|^4\}\,. \tag{3.21b}$$

It is evident that for the particular choice $\alpha = 0, \beta \neq 0$ we may recover from (3.21a) and (3.21b) the well-known relations due to Lakshmanan.[1]

The parameters in Eq. (3.18) are simplified in the following particular cases:

$$\epsilon = 1\,, \quad \text{for} \quad \alpha = 0\,, \quad \beta \neq 0 \quad \text{and} \quad \alpha \neq 0\,, \quad \beta = 0\,,$$
$$\gamma = \begin{cases} +4\sqrt{2\beta}\,\lambda_0\,, & \text{for} \quad \alpha = 0\,, \quad \beta \neq 0\,, \\ -4\alpha\lambda_0^2\,, & \text{for} \quad \alpha \neq 0\,, \quad \beta = 0\,, \end{cases} \tag{3.22}$$

$$\rho=\begin{cases}0, & \text{for } \alpha=0,\ \beta\neq 0,\\ \dfrac{1}{4\alpha\lambda_0^2}, & \text{for } \alpha\neq 0,\ \beta=0,\end{cases}$$

and $d=e=0$ for both $\alpha=0,\beta\neq 0$ and $\alpha\neq 0,\beta=0$. Note that the case $\alpha=0,\beta\neq 0$ yields standard NSE (3.1) from MNS (3.10) and similarly $\alpha\neq 0,\beta=0$ gives DNS (3.3). It is also immediate from (3.22) that MLL (3.18) reduces successively to LLE (3.2) and DLL (3.9) in these respective cases. The energy and current density relations (3.21) are also simplified accordingly.

D. MDLL gauge generated from MDNS

The modified derivative nonlinear Schrödinger equation (MDNS) proposed in Ref. 12 is given by

$$q_t-i(q/\Phi)_{xx}=0,\quad \Phi=(1\pm|q|^2)^{1/2}, \tag{3.23}$$

which corresponds to the linear system (2.1b) with

$$U=-i\lambda\sigma_3+\lambda A,$$
$$V=2\lambda^2 D+\lambda B, \tag{3.24}$$

where A is as in (3.5) and

$$B=i\begin{pmatrix}0, & (q/\Phi)_x\\ \pm(q^*/\Phi)_x, & 0\end{pmatrix},\quad D=\Phi^{-1}\begin{pmatrix}-i, & q\\ \pm q^*, & i\end{pmatrix}. \tag{3.25}$$

Repeating the above procedure we get the gauge-transformed operators as

$$U'=(\lambda-\lambda_0)g^{-1}\{-i\sigma_3+A\}g,$$
$$V'=g^{-1}\{2(\lambda^2-\lambda_0^2)D+(\lambda-\lambda_0)B\}g. \tag{3.26}$$

From (2.9) and (2.10) we deduce the relations

$$SS_x=2\lambda_0 g^{-1}Ag, \tag{3.27a}$$
$$(1/2\lambda_0)S(S_t-2\lambda_0\chi S_x)=g^{-1}Bg,$$
$$\chi=(1+\mathrm{tr}(S_x^2)/8\lambda_0^2)^{-1/2}, \tag{3.27b}$$

and

$$\chi S((1/2\lambda_0)S_x-i)=g^{-1}U_0(-\mathrm{tr}(U_0^2)/2)^{-1/2}g=g^{-1}Dg. \tag{3.27c}$$

Where the relation $D=U_0(-\mathrm{tr}(U_0^2)/2)^{-1/2}$ has been used. Using (3.27) we get finally from (3.26)

$$U'=(\lambda-\lambda_0)(-iS+(1/2\lambda_0)SS_x),$$
$$V'=2(\lambda^2-\lambda_0^2)\chi S((1/2\lambda_0)S_x-i\bar{I})$$
$$+(\lambda-\lambda_0)S(S_t-2\lambda_0\chi S_x)/2\lambda_0, \tag{3.28}$$

which yields the following modified derivative Landau–Lifshitz (MDLL) type equation gauge equivalent to MDNS:

$$S_t=i(\chi SS_x)_x+4\lambda_0\chi S_x, \tag{3.29}$$

with $S\in$SU(2)/U(1) [SU(1,1)/U(1)] corresponding to $+(-)$ signs in (3.23).

IV. HIGHER-ORDER NS TYPE SYSTEMS

We show that from nonlinear Schrödinger (NS) type systems one may generate through U(1)-gauge transformations some new higher-order nonlinear equations, which will also be integrable due to their gauge equivalence with integrable NS systems. If we start with the MNS (3.10), then it is not difficult to find that under the U(1)-gauge transformation

$$h=\begin{pmatrix}e^{i\Theta}, & 0\\ 0, & e^{-i\Theta}\end{pmatrix}$$

the linear operators change to a new system giving the equation

$$(iQ_t+Q_{xx}\pm i\alpha(|Q|^2Q)_x\pm\beta|Q|^2Q$$
$$+2(\Theta_t-2\Theta_x^2-i\Theta_{xx})Q$$
$$-2\Theta_x(2iQ_x\mp 2|Q|^2Q)=0, \tag{4.1}$$

where the new field $Q=qe^{2i\Theta}$ has been introduced choosing

$$\Theta_x=\mp\delta|q|^2, \tag{4.2a}$$

and

$$\Theta_t=\pm i\delta(qq^*_x-q^*q_x)+\tfrac{3}{2}\alpha\delta|q|^4, \tag{4.2b}$$

Eq. (4.1) reduces to a higher-order MNS (named HMNS) given by

$$iQ_t+Q_{xx}\pm i\alpha(|Q|^2Q)_x\pm\beta|Q|^2Q+\delta(4\delta+\alpha)|Q|^4Q$$
$$\pm 4i\delta(|Q|^2)_xQ=0. \tag{4.3}$$

Note that Eqs. (4.2) are consistent with the condition $\Theta_{xt}=\Theta_{tx}$ due to Eq. (3.10), and (4.2a) and (4.2b) are, respectively, the densities of first ("particle number") and second ("current") conservation laws for system (3.10).

For the particular case $\alpha=0,\beta\neq 0$, which reduces MNS to the standard NSE (3.1), one gets the corresponding higher-order system (named HNS) through gauge transformation (4.2) in the form

$$iQ_t+Q_{xx}\pm\beta|Q|^2Q+4\delta^2|Q|^4Q\pm 4i\delta(|Q|^2)_xQ=0. \tag{4.4}$$

Equation (4.4) may also be obtained directly from (4.3) by putting $\alpha=0$.

The case $\alpha\neq 0,\beta=0$ on the other hand reduces MNS to DNS (3.3). The U(1)-gauge transformation (4.2), therefore, generates from DNS the following higher-order equation (named HDNS), which is also obtainable from (4.3) for $\beta=0$:

$$iQ_x+Q_{xx}\pm i\alpha(|Q|^2Q)_x+\delta(4\delta+\alpha)|Q|^4Q$$
$$\pm 4i\delta(|Q|^2)_xQ=0. \tag{4.5}$$

It is remarkable that the particular choice $\alpha=-4\delta$ leads further (4.5) to the Chen–Lee–Liu (CLL)[13] equation

$$iQ_t+Q_{xx}+i\alpha|Q|^2Q_x=0, \tag{4.6}$$

whereas the choice $\alpha=-2\delta$ transforms (4.5) to the Gerdjikov–Ivanov first type (GI_1) equation

$$iQ_t+Q_{xx}+2\delta^2|Q|^4Q\pm 2i\delta Q^2Q^*_x=0. \tag{4.7}$$

Thus, all the equations (4.5)–(4.7) are gauge equivalent to DNS (3.3), the connection between the spectral problems of CLL and DNS found recently by Wadati and Sogo[16] reflects, as shown here, a more general gauge equivalence between them.

If, however, we set $\alpha=-4\delta,\beta\neq 0$, (4.3) yields a mixed CLL and NSE type equation (denoted by CLL–NS)

$$iQ_t+Q_{xx}\pm\beta|Q|^2Q\pm i\alpha|Q|^2Q_x=0, \tag{4.8}$$

while for $\alpha=-2\delta,\beta\neq 0$, we get the Gerdjikov–Ivanov second type (GI_2) equation

$$iQ_t+Q_{xx}\pm\beta|Q|^2Q\pm 2\delta^2|Q|^4Q\pm 2i\delta Q^2Q^*_x=0. \tag{4.9}$$

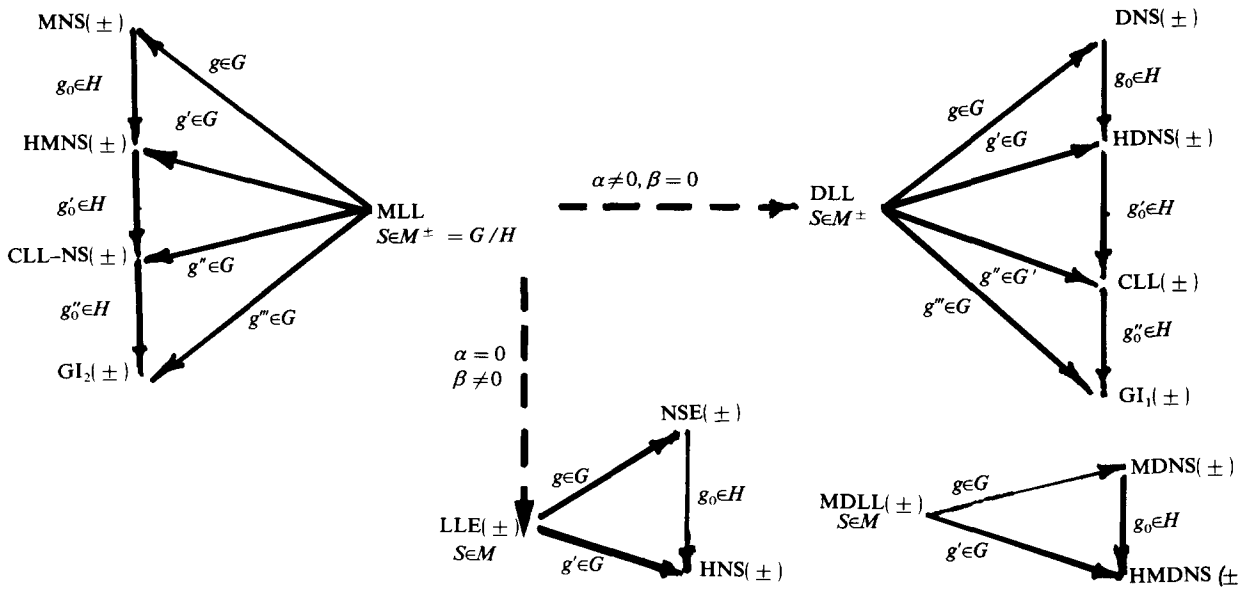

FIG. 1. Gauge equivalence between various LLE and NS systems. The LLE with field $S \in M^{\pm} = G/H$, where $H = \mathrm{U}(1)$, $G = \mathrm{SU}(2)$, and $\mathrm{SU}(1,1)$, corresponds, respectively, to the "attractive" (+) and "repulsive" (−) types of NS systems.

Therefore, equations (4.3), (4.8), and (4.9) are naturally gauge-connected with MNS (3.10). Similarly, from MDNS (3.23) by h-gauge transformation $\Theta_x = \alpha\Phi$ and $\Theta_t = \pm \alpha i \Phi^{-2}(q^* q_x - q_x^* q)$ one gets a higher-order nonlinear equation (called HMDNS) in the form

$$iQ_t + (Q/\Phi)_{xx} - 2\alpha i Q_x(1 + \Phi^{-2}) - 4\alpha^2 Q/\Phi = 0 . \tag{4.10}$$

Frequently, in solving practical problems, higher-order nonlinear terms are neglected to approximate the field equation to some integrable system. The examples presented here demonstrate however that often the higher-order nonlinear equations are reducible exactly to some standard integrable system through gauge transformation without neglecting any higher nonlinearities.

V. GAUGE EQUIVALENCE BETWEEN VARIOUS LLE AND NS SYSTEMS

If G is the connected Lie group associated with Landau–Lifshitz systems and $H \subset G$ is the closed subgroup of G, then the corresponding field function $S \in G/H$ under local gauge transformation $g(x) \in G$ may be represented as $S = g^{-1}\Sigma g$, where Σ is a diagonal matrix with $[\Sigma, h] = 0$, $h \in H$ (see Ref. 7). Such gauge transformations (as shown in Sec. III) change the LLE to the corresponding NS system. Note now that the gauge transformation $g \to g' = hg$ with $h(x) \in H$ keeps the S field left-invariant $S' = (g')^{-1}\Sigma g' = g^{-1}\Sigma g = S$. Similarly, S is right-invariant ($g' = gh$) for the representation $S = g\Sigma g^{-1}$. Consequently, under $[h(x) \in H]$-transformation LLE is invariant, while the NS system may change. We conclude, therefore, that together with different NSE all their gauge-transformed equations relative to local group H or any subgroup of it are also gauge equivalent to the corresponding LLE systems.

Hence, in light of the $[H = \mathrm{U}(1)]$-invariance of the LLE, we find the diagram (Fig. 1) of gauge equivalence between LLE and NS systems proposed here.

VI. CONCLUDING REMARKS

We have found a number of LLE systems through gauge transformation of known NS type equations. By U(1)-gauge transformation of NS systems we have also generated different higher-order nonlinear equations. Due to the gauge equivalence with integrable NSE the integrability property of the proposed systems may be predicted. Therefore, such nonlinear systems might be of much use for approximating some real models in quasi-one-dimension.

The nonlinear equations proposed here may be generalized also for higher-order compact or noncompact groups,[7] e.g., $G = \mathrm{SU}(p+q)$, $H = S(\mathrm{U}(p) \times \mathrm{U}(q))$ or $G = \mathrm{SU}(p,q)$, $H = S(\mathrm{U}(r,u) \times \mathrm{U}(s,v))$ with $r + s = p$ and $u + v = q$. The generalized LLE systems with $S \in G/H$ would be gauge equivalent to the corresponding matrix NS systems with global symmetry group H and to all their gauge-transformed entities relative to the local group H or to any of its subgroups.

We conclude with the remark that, usually for gauge transformation, Jost functions are taken at $\lambda = \lambda_0 = 0$. Here, in finding gauge equivalence of different NS systems, one as a rule must choose $\lambda_0 \neq 0$.

ACKNOWLEDGMENTS

The author would like to extend his thanks to Professor V. Makhankov of JINR for interest in this work.

He would also like to thank the Directorate of the Joint Institute for Nuclear Research, Dubna, USSR for the offer of a Research Associateship position.

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Generalized logarithmic Borel summability

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(Received 20 December 1983; accepted for publication 15 June 1984)

The recently introduced logarithmic Borel summation method is able to sum strongly divergent series of a particular type. A satisfactory extension to the applicability of this method, obtained by using the classical Borel–Le Roy transform, is presented. As examples we consider a class of nonpolynomial anharmonic oscillator models in the 't Hooft simplified form.

PACS numbers: 02.30.Lt

I. INTRODUCTION

It is well known that most of the classical applications of the Rayleigh–Schrödinger perturbative theory, such as the Stark–Lo Surdo effect, the Zeeman effect, and anharmonic oscillators (for a review see, e.g., Refs. 1 and 2) give rise to diverging power-series expansions. In all such problems we have eigenvalues or resonances with asymptotic power-series expansions given by the perturbative theory $E_n(\beta) \sim \Sigma_k a_k^{(n)} \beta^k$ as $\beta \neq 0$.

An important result in mathematical physics is the proof that an eigenvalue (or a resonance) can be actually obtained from the perturbative series by the Borel sum.[3–5]

More singular perturbations of solvable quantum mechanical Hamiltonians have been recently studied, showing the failure of the classical Borel summability. An example is given by the exponential anharmonic oscillator with Hamiltonian $p^2 + x^2 + \beta e^{\sqrt{\alpha} x}$, $\alpha \in \mathbb{R}^+$ (see Refs. 6 and 7). In such cases we expect power-series coefficients diverging as $e^{\alpha k^2/4}$ (see Ref. 6).

A method of sum called "logarithmic Borel," which is able to treat such a diverging series, has been previously proposed.[8] Now we present a class of generalized Borel summation methods of order (α,m), $\alpha \in [0,\infty)$, $m = 0, 1, 2, \ldots$, that contains the previous ones as particular cases. It is able to sum series with coefficients a_k diverging as $(mk)! e^{\alpha k^2/4}$.

Possible physical examples are given by mixed power-exponential anharmonic oscillators like $H = p^2 + x^2 + \beta x^n e^{\sqrt{\alpha} x}$, $n \in \mathbb{N}$. Another possible application is the high-temperature power-series expansion of the pressure for a classical gas with a smooth pair interaction potential $\Phi(|x_i - x_j|)$ such that $\Phi(r) \sim \exp((\ln r^{-1})^{1/2})$ as $r \to 0$ (for less singular potentials and usual Borel summability see Ref. 9). In Sec. II the summability criterion and the necessary condition theorem are proved for $\alpha > 0$, $m \in \mathbb{N}$. In Sec. III we apply the criterion to a class of simplified physical examples. In the Appendix we give the asymptotic behavior of the weight functions appearing in the direct and inverse Borel transforms.

II. THE METHODS

Each one of the methods we consider is a particular case of the "moment constant methods" (Ref. 10, pp. 81–86) for which we are able to give a criterion of the Watson–Nevanlinna type (see Ref. 10, pp. 192–195, and Refs. 11 and 12). Thus let us recall the "moment constant methods."

Let $\rho(x) > 0$ be a function defined on $\mathbb{R}^+$ with finite moments $\mu_k = \int_0^\infty x^k \rho(x) dx$, $k = 0, 1, 2, \ldots$. We say that a series $\Sigma_k a_k z^k$ is μ-ρ-Borel summable if (a) $B(v) = \Sigma_{k=0}^\infty a_k (\mu_k)^{-1} v^k$ is convergent in some disk $|v| < d$; (b) $B(v)$ has an analytic continuation to a neighborhood of the positive real axis; (c) $f(z) = z^{-1} \int_0^\infty B(v) \rho(vz^{-1}) dv$ converges for some $z > 0$. Notice that if $\rho(x)$ is analytic, $f(z)$ can be defined for nonreal values of z as well. In such a case $f(z)$ is the μ-ρ-Borel sum of $\Sigma_k a_k z^k$ and $B(v)$ is the μ-ρ-Borel transform.

We now consider a class of ρ functions classified by two parameters (α,m) and we call $f(z)$ the (α,m) Borel sum of the series if $\rho = \rho_{(\alpha,m)}$ is given by the following.

$$\text{(i)}\ \rho_{(\alpha,m)}(x) = (\pi\alpha)^{-1/2} (mx)^{-1} \int_0^\infty \exp(-\alpha^{-1} (\ln(xt))^2 - t^{-1/m}) t^{-1-1/m} dt$$

for $\alpha > 0$, $m = 1, 2, 3, \ldots$.

$$\text{(ii)}\ \rho_{(\alpha,m)}(x) = (\pi\alpha)^{-1/2} x^{-1} \exp(-\alpha^{-1} (\ln(x))^2)$$

for $\alpha > 0$, $m = 0$.

$$\text{(iii)}\ \rho_{(\alpha,m)}(x) = m^{-1} e^{-x^{1/m}} x^{-1+1/m}$$

for $\alpha = 0$, $m = 1, 2, 3, \ldots$.

The classification is justified by the behavior of the moments

$$\mu_k(\alpha,m) = \int_0^\infty x^k \rho_{(\alpha,m)}(x) dx = (mk)! e^{\alpha k^2/4}.$$

The case (iii) is the usual Borel–Le Roy summation.[5,10] Let us state the criterion for the logarithmic Borel summability (ii)[8] and for the generalized logarithmic Borel summability (i) together.

Theorem 1: Let $m \in \mathbb{N}_0$, $\alpha \in \mathbb{R}^+$. Let $f(z)$ be an analytic function on the Riemann surface of $\ln(z)$ in a domain D given by

$$D = \{z / -\infty < \mathrm{Re}(\ln(z)) < c_0\} \text{ for some } c_0 \in \mathbb{R},$$

satisfying the following properties:

$$f(z) = \sum_{k=0}^{N-1} a_k z^k + R_N(z), \tag{1}$$

$$|R_N(z)| \leqslant A(|\theta|) b_N |z|^N, \quad N \in \mathbb{N},\ z \in D, \tag{2}$$

where $\theta = \arg(z)$, $A(\phi) = e^{\alpha^{-1}(\phi - m\pi/2 - \epsilon)^2}$ for some $\epsilon > 0$, and $b_N = (mN)! \delta^N e^{\alpha N^2/4}$, $N = 1, 2, \ldots$, where A, δ, ϵ are inde-

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pendent of z. Then the series $\Sigma_k a_k z^k$ is (α,m) Borel summable to $f(z)$.

Proof: The $m = 0$ case is proved in Ref. 8. All the $m > 0$ cases reduce to the $m = 1$ by an argument exposed in Remark 1, so it is sufficient to prove the $(\alpha,1)$ Borel summability. Let $\rho(w)$, $\sigma(w)$ be defined by

$$\rho(w) = \rho_{(\alpha,1)}(w) = (\alpha\pi)^{-1/2} w^{-1} \int_0^\infty \exp(-\alpha^{-1}(\ln wt)^2 - t^{-1}) t^{-2}\, dt, \tag{3}$$

$$\sigma(w) = 2(\alpha\pi)^{1/2}(2\pi i)^{-1} \oint_{\gamma(r,\epsilon_1)} \exp(\alpha^{-1}(\ln wt)^2 + t^{-1}) t^{-1}\, dt, \tag{4}$$

where $\gamma(r,\epsilon_1) = \{t/|t| = r,\ |\arg(t)| \leqslant \epsilon_1 + \pi/2\} \cup \{t/\arg(t) = \pm(\epsilon_1 + \pi/2),\ |t| \leqslant r\}$. Of course the integral (4) is independent of r and ϵ_1 for $r \in \mathbb{R}^+$ and $0 < \epsilon_1 < \pi/2$. The functions ρ and σ enjoy the following asymptotic behaviors:

$$\rho(w) = w^{-1} \exp\{-\alpha^{-1}(\ln w\alpha/2)^2 + 2\alpha^{-1}(\ln w\alpha/2)(\ln\ln w\alpha/2) - 2\alpha^{-1}\ln w\alpha/2 + O((\ln\ln w\alpha/2)^2)\}, \tag{5}$$

$$\sigma(w) = \exp\{\alpha^{-1}(\ln w\alpha/2)^2 - 2\alpha^{-1}(\ln w\alpha/2)(\ln\ln w\alpha/2) + 2\alpha^{-1}\ln w\alpha/2 + O((\ln\ln w\alpha/2)^2)\} \tag{6}$$

as $w \to \infty$ in any finite sector of the Riemann surface of $\ln w$ (for a proof see the Appendix).

Set $z = |z|e^{i\theta}$, $v = |v|e^{i\psi}$, $t = |t|e^{i\phi}$. For $|\psi| < \epsilon$ and $j = 0, 1, 2, \ldots$ let us define

$$B^{(j)}(v) = (2\pi i\alpha)^{-1} \int_{-i\infty+c}^{+i\infty+c} f(e^u) \frac{\partial^j}{\partial v^j} \sigma(ve^{-u}) du, \tag{7}$$

where $u = \ln z$ varies along the axis $\mathrm{Re}\, u = c$, and the integral is independent of c, $c \in (-\infty, c_0)$. The integral in (7) is absolutely convergent and defines the jth derivative of $B(v) = B^{(0)}(v)$,

$$\begin{aligned} |B^{(j)}(v)| &= \left| (2\pi i\alpha)^{-1} \int_{-i\infty+c}^{+i\infty+c} f(e^u) \frac{(\pi\alpha)^{1/2}}{(\pi i)} \oint_{\gamma(r,\epsilon_1)} e^{v/t} e^{\alpha^{-1}(u - \ln t)^2} t^{-1-j}\, dt\, du \right| \\ &\leqslant D_0 \int_{-\infty}^{+\infty} |f(e^{c+i\theta})| \left(2\int_0^r \exp(|v|\tau^{-1}\cos(\epsilon_1 - |\psi| + \pi/2)) e^{\alpha^{-1}(c - \ln\tau)^2} \exp(-\alpha^{-1}(\epsilon_1 - |\theta| + \pi/2)^2) \tau^{-1-j}\, d\tau \right. \\ &\quad \left. + \int_{-\epsilon_1 - \pi/2}^{+\epsilon_1 + \pi/2} e^{|v|r^{-1}} r^{-1-j} e^{\alpha^{-1}(c - \ln r)^2} e^{-\alpha^{-1}(\theta - \phi)^2}\, d\phi \right) d\theta, \end{aligned} \tag{8}$$

where the integral in τ exists if $|\psi| < \epsilon_1 < \epsilon$, so that also by the bound $|f(e^{c+i\theta})| \leqslant A' e^{\alpha^{-1}(|\theta| - \epsilon - \pi/2)^2}$, implicit in (2), it follows that $B(v)$ is analytic in the whole sector $|\arg(v)| < \epsilon$.

On the other hand, by inserting (1) into (7) (for $j = 0$) we have

$$B(v) = (2\pi i\alpha)^{-1} \left(\int_{-i\infty+c}^{+i\infty+c} \sum_{k=0}^{N-1} a_k e^{ku} \sigma(ve^{-u}) du + \int_{-i\infty+c}^{+i\infty+c} R_N(e^u) \sigma(ve^{-u}) du \right). \tag{9}$$

By interchanging the order of integration and performing the Gaussian integral, the first term in (9) turns out to be

$$\begin{aligned} &\frac{(\pi\alpha)^{-1/2}}{(2\pi i)} \oint_{\gamma(r,\epsilon_1)} e^{\alpha^{-1}(\ln vt)^2 + t^{-1}} t^{-1} \int_{-\infty}^{+\infty} \sum_{k=0}^{N-1} a_k \exp((c + i\theta)(k - 2\alpha^{-1}\ln vt)) e^{\alpha^{-1}(c + i\theta)^2}\, d\theta\, dt \\ &= \sum_{k=0}^{N-1} a_k e^{-\alpha k^2/4} (2\pi i)^{-1} \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} (vt)^k e^{t^{-1}} t^{-1}\, dt = \sum_{k=0}^{N-1} a_k (k!\, e^{\alpha k^2/4})^{-1} v^k. \end{aligned} \tag{10}$$

Therefore, by (9), (10), and (2) we have

$$\begin{aligned} &\left| B(v) - \sum_{k=0}^{N-1} a_k (k!\, e^{\alpha k^2/4})^{-1} v^k \right| \\ &= \left| \frac{2(\pi\alpha)^{1/2}}{(2\pi i)^2 \alpha} \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} e^{vt^{-1}} t^{-1} \int_{-i\infty+c}^{+i\infty+c} R_N(e^u) e^{\alpha^{-1}(u - \ln t)^2}\, du\, dt \right| \\ &= \left| \frac{2(\pi\alpha)^{1/2}}{(2\pi i)^2 \alpha} \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} e^{vt^{-1}} t^{-1} \int_{-i\infty+c'}^{+i\infty+c'} e^{\alpha^{-1}(w^2 - 2i\phi w - \phi^2)} R_N(e^{w + \ln|t|})\, dw\, dt \right| \\ &\quad \text{[where } w = u - \ln|t|\text{, and } c' \text{ can vary in } (-\infty, c_0) \text{ if } 2r \leqslant 1\text{]} \\ &\leqslant A \left| \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} e^{vt^{-1}} t^{-1} \int_{-\infty}^{+\infty} e^{\alpha^{-1}(c'^2 - (\theta - \phi)^2)} \exp(\alpha^{-1}(\theta^2 - 2(\epsilon + \pi/2)|\theta|)) e^{Nc' + \alpha N^2/4} N!\, \delta^N |t|^N\, d\theta\, dt \right| \\ &\quad \text{(by choosing } c' = -N\alpha/2\text{, since } |\phi| \leqslant \epsilon_1 + \pi/2 < \epsilon + \pi/2\text{)} \\ &\leqslant A_1 \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} \delta^N |e^{vt^{-1}} t^{-1} N!\, t^N\, dt| \leqslant A_2 \delta^N N^{1/2} v^N \end{aligned} \tag{11}$$

(by choosing $r = v/N$). So, for all v such that $0 < v < \delta^{-1}$ the remainder tends to zero as $N \to +\infty$. On the other hand the power-series expansion for $B(v)$ near $v = 0$ is just convergent in the disk $|v| < \delta^{-1}$ by (10) and by the bound $|a_k| \leqslant A_3 \delta^k (k!) e^{\alpha k^2/4}$ implicit in (2). Thus, $B(v)$ defines an analytic function in the region $S(\delta,\epsilon) = \{v/|v| < \delta^{-1} \text{ or } |\arg(v)| < \epsilon\}$, and it is uniquely determined by the a_k's. Besides, for large $|v|$, $B(v)$ can be bounded by means of the estimate (6) on $\sigma(w)$

$$
\begin{aligned}
|B(v)| \leqslant A_4 \int_{-\infty}^{+\infty} \Big| e^{\alpha^{-1}(|\theta| - \epsilon - \pi/2)^2} \exp\Big\{ & \alpha^{-1}\Big(\ln \frac{|v|\alpha}{2e^c} + i(\psi - \theta)\Big)^2 \\
& + 2\alpha^{-1}\Big(\ln \frac{|v|\alpha}{2e^c} + i(\psi - \theta)\Big) - 2\alpha^{-1}\Big(\ln \frac{|v|\alpha}{2e^c} + i(\psi - \theta)\Big)\ln\Big(\ln \frac{|v|\alpha}{2e^c} + i(\psi - \theta)\Big) + O\Big(\ln\ln \frac{|v|\alpha}{2e^c}\Big)^2 + o(\theta)\Big\} \Big| d\theta \\
\leqslant A_4 \Big(\int_{-\infty}^{+\infty} & e^{-2\alpha^{-1}(\epsilon + \pi/2)|\theta|} e^{2\alpha^{-1}\psi\theta}\, e^{2\alpha^{-1}(\psi - \theta)\pi/2} e^{o(\theta)} d\theta \Big) \exp\Big\{ \alpha^{-1}\Big(\ln \frac{|v|\alpha}{2e^c}\Big)^2 \\
& + 2\alpha^{-1} \ln \frac{|v|\alpha}{2e^c} - 2\alpha^{-1}\Big(\ln \frac{|v|\alpha}{2e^c}\Big)\Big(\ln\ln \frac{|v|\alpha}{2e^c}\Big) + O\Big(\ln\ln \frac{|v|\alpha}{2e^c}\Big)^2 \Big\},
\end{aligned}
\tag{12}
$$

where the integral is convergent (and independent of $|v|$) for $|\arg(v)| = |\psi| < \epsilon$, and the estimate is correct for all $c \in (-\infty, c_0)$. By the analyticity of $B(v)$ in $S(\delta,\epsilon)$, by the bound (12) for large $|v|$, and by (5) we have, for any ψ and ϕ such that $|\psi| < \epsilon$, $|\phi| \leqslant \pi/2$:

$$
\begin{aligned}
\Big| z^{-1} \int_0^{\infty} B(ve^{i\psi}) \rho(ve^{i\psi} z^{-1}) e^{i\psi}\, dv \Big| \leqslant & \int_0^1 v^{-1} \int_0^{\infty} |\exp - (\alpha^{-1}(\ln ve^{i\psi} te^{i\phi} z^{-1})^2) e^{-i\phi} t^{-2}\, dt\, B(ve^{i\psi})| dv \\
& + e^{\alpha^{-1}(\psi - \theta)^2} \int_1^{\infty} v^{-1} \exp\Big\{ 6\alpha^{-1}\Big(\ln \frac{v\alpha}{2}\Big)(\ln|z| - c) - \alpha^{-1}(\ln|z|)^2 + \alpha^{-1}c^2 \\
& + 2\alpha^{-1}\Big(\ln \frac{v\alpha}{2|z|}\Big)\Big(\ln\ln \frac{v\alpha}{2|z|}\Big) \mp 2\alpha^{-1}\theta\pi/2 - 2\alpha^{-1}\Big(\ln \frac{v\alpha}{2e^c}\Big)\Big(\ln\ln \frac{v\alpha}{2e^c}\Big) \\
& + O(\ln\ln v)^2 + o(\theta)\Big\} dv \leqslant A_5 e^{o(\theta)} \{ e^{\alpha^{-1}(\psi + \phi - \theta)^2} \\
& + e^{-\alpha^{-1}(\ln|z|)^2} \exp(2\alpha^{-1}(\ln|z|^{-1})(\ln\ln|z|^{-1})) \exp\{\alpha^{-1}(\psi - \theta)^2 \mp 2\alpha^{-1}\theta\pi/2)\},
\end{aligned}
\tag{13}
$$

if only c is chosen such that $\ln|z| - c < 0$ (which can be done uniformly for $|z|$ small). Notice that (13) holds for $0 < |z| < e^{c_0}$ for any ψ and ϕ such that $|\psi| < \epsilon$, $|\phi| \leqslant \pi/2$; and with $(-\pi/2)$ in the second term if $\theta > 0$ and $(+\pi/2)$ if $\theta < 0$. So, by suitably choosing ψ and ϕ,

$$
\Big| z^{-1} \int_0^{\infty} \rho(v/z) B(v) dv \Big| \leqslant A_6 \exp(\alpha^{-1}(|\theta| - \pi/2 - \epsilon_0)^2)
\tag{14}
$$

uniformly for any fixed $\epsilon_0 < \epsilon$, for $z \in D$, for some A_6 independent of z. In particular, the integral in (14) is absolutely convergent. One can verify that it equals the function $f(z)$ by interchanging the order of integration and performing the two integrals as a logarithmic Borel sum, whose transform is not regular in the origin, but is a Borel sum:

$$
z^{-1} \int_0^{\infty} \rho(v/z) B(v) dv = (\alpha\pi)^{-1/2} \int_0^{\infty} e^{-\alpha^{-1}(\ln t/z)^2} \Big(t^{-1} \int_0^{\infty} e^{-v/t} B(v) dv \Big) t^{-1}\, dt.
\tag{15}
$$

Alternatively, one can perform two Laplace transformations in the right-hand side of (15), while $B(v)$ given by (7) can be computed showing the corresponding inversion formulas

$$
\begin{aligned}
B(v) = (2\pi i)^{-1} & \oint_{\mathrm{Re}\, t^{-1} = r^{-1}} e^{v/t} t^{-1} 2(\pi\alpha)^{1/2} (2\pi i\alpha)^{-1} \\
& \times \int_{-i\infty + c}^{+i\infty + c} e^{\alpha^{-1}(u - \ln t)^2} f(e^u) du.
\end{aligned}
\tag{16}
$$

Thus inserting (16) into (15) we have an identity and the criterion is proved.

From assumptions (1) and (2) it actually follows that the generalized Borel transform $B(v)$ is analytic for $v \in S(\delta,\epsilon) \equiv \{v/|v| < \delta^{-1} \text{ or } |\arg(v)| < \epsilon\}$ and satisfies a bound of the type (12) uniformly on each $S(\delta_1,\epsilon_1)$ with $\delta_1 > \delta$, $\epsilon_1 < \epsilon$. In view of Remark 1, such a bound is easily extended to any case with $m \in \mathbb{N}$: Indeed, by replacing α by αm^{-2} and v by $v^{1/m}$ one checks (17). In the following theorem we assume such properties of $B(v)$ and we prove that (1) and (2) are necessary conditions too for generalized logarithmic Borel summability.

Theorem 2: Let $B(v)$ be an analytic function in $S(\delta,\epsilon) = \{v/|v| < \delta^{-1} \text{ or } |\arg(v)| < \epsilon\}$, satisfying

$$
\begin{aligned}
|B(v)| \leqslant \exp\{ & m^2\alpha^{-1}(\ln \alpha|v|^{1/m}/2m^2e^c)^2 \\
& + 2m^2\alpha^{-1} \ln(\alpha|v|^{1/m}/2m^2e^c) \\
& - 2m^2\alpha^{-1}(\ln \alpha|v|^{1/m}/2m^2e^c)(\ln\ln \alpha|v|^{1/m}/2m^2e^c) \\
& + O(\ln\ln \alpha|v|^{1/m}/2m^2e^c)\}
\end{aligned}
\tag{17}
$$

for all $c \in (-\infty, c_0)$, uniformly on $S(\delta_1,\epsilon_1)$ for any $\delta_1 > \delta$, $\epsilon_1 < \epsilon$. Then the function

$$
f(z) = z^{-1} \int_0^{\infty} \rho_{(\alpha,m)}(vz^{-1}) B(v) dv
$$

is analytic in the domain D of Theorem 1 and satisfies condi-

tions of the type (1) and (2), where A, δ, ϵ are, respectively, replaced by some A_0, $\delta_0 > 0$, and by any $\epsilon_0 < \epsilon$.

Proof: Without loss of generality we can treat the $(\alpha,1)$ case (see Remark 1). Let $B(v)$ satisfy (17), with $m = 1$, and analyticity in $S(\delta,\epsilon)$. Then, in analogy with (13), one checks that $f(z)$ exists and is analytic for $z \in D$. Moreover, for values of ψ and ϕ to be specified, we have

$$f(z) - \sum_{k=0}^{N-1} a_k z^k = \int_0^\infty \left[B(ve^{i\psi}) - \sum_{k=0}^{N-1} a_k (k!e^{\alpha k^2/4})^{-1} (ve^{i\psi})^k \right] (\alpha\pi)^{-1/2} \times \int_0^\infty e^{-\alpha^{-1}(\ln te^{i\phi}/z)^2} t^{-2} e^{-i\phi} e^{-ve^{\alpha\psi - \phi)}/t}\, dt\, dv. \quad (18)$$

It is sufficient to bound the integral in v near $v = 0$, since at $v = \infty$ the estimate is analogous to the one in (13) and it gives just

$$D_0 e^{-\alpha^{-1}(\ln|z|)^2} \exp(2\alpha^{-1}(\ln|z|^{-1})(\ln\ln|z|^{-1})) \times \exp(\alpha^{-1}(|\theta| - \pi/2 - \epsilon_0)^2) \quad (19)$$

for some $D_0 > 0$, for any $\epsilon_0 < \epsilon$.

Near $v = 0$ we have

$$\int_0^\infty |\exp(-\alpha^{-1}(\ln tz^{-1}e^{-i\phi})^2) t^{-2}| \times \int_0^{\delta^{1/2}} (D_1)^N v^N e^{-vt^{-1}\cos(\psi - \phi)}\, dv\, dt \leqslant (D_2)^N (N!) |z|^N e^{\alpha N^2/4} e^{\alpha^{-1}(\phi - \theta)^2} \quad (20)$$

if $\cos(\psi - \theta) > 0$, that is $|\psi - \theta| < \pi/2$. By suitably choosing ψ and ϕ ($\phi = \epsilon_0 + \pi/2$, $\psi = \epsilon_1$, where $\epsilon_0 < \epsilon_1 < 0$ if $\theta > 0$; $\phi = -\epsilon_0 - \pi/2$, $\psi = -\epsilon_1$ if $\theta < 0$) we have from (19) and (20)

$$|R_N(z)| \leqslant A_0(\delta_0)^N (N!) e^{\alpha N^2/4} |z|^N \exp(\alpha^{-1}(|\theta| - \pi/2 - \epsilon_0)^2)$$

uniformly for any fixed $\epsilon_0 > \epsilon$ and the theorem is proved.

Remark 1: Let $f(z)$ satisfy the condition of Theorem 1 with parameters (α,m), $m > 1$, $\alpha > 0$. If we consider $\phi(z) = f(z^m)$ we have $\phi(z)$ satisfying conditions of the type (1) and (2) with parameters $(\alpha m^{-2},1)$ on D. Since Theorem 1 is proved for $m = 1$, the Borel transform $\tilde{B}(w)$ exists and $\phi(z)$ is given by

$$\phi(z) = z^{-1} \int_0^\infty \tilde{B}(w) \rho_{(\alpha m^{-2},1)}(wz^{-1}) dw. \quad (21)$$

By the relation $\rho_{(\alpha m^{-2},1)}(x) = x^{m-1} \rho_{(\alpha,m)}(x^m)$, $f(z)$ is the (α,m) Borel sum,

$$f(z) = z^{-1} \int_0^\infty B(v) \rho_{(\alpha,m)}(vz^{-1}) dv, \quad (22)$$

where $B(v) = m^{-1}\tilde{B}(v^{1/m})$. So the criterion is proved for $\alpha > 0$, $m > 1$. Since (21) and (22) are equivalent, the argument can be reversed and Theorem 2 is proved for all $\alpha > 0$, $m > 1$, too.

III. APPLICATION

To give a physical example in which Theorem 1 can be applied, let us consider the trace of the semigroup generated by $H(\beta) = p^2 + x^2 + \beta x^{m+1} e^x$: $\mathrm{Tr}(e^{-tH(\beta)})$, $t \geqslant 0$, $\beta > 0$. We examine a simplified model, suggested by 't Hooft, in which the integral kernel K of $e^{-tH(\beta)}$ is replaced by $K^{(1)}$, where the $K^{(n)}$'s are the approximating kernels in Trotter formula.[13] In the notation of Ref. 13 the trace corresponding to $K^{(1)}$ is given by

$$T_t(\beta) = \int_{-\infty}^{+\infty} K^{(1)}(x,x; -it)dx = \int_{-\infty}^{+\infty} (2\pi t)^{-1/2} e^{-t(x^2 + \beta x^{m+1} e^x)}\, dx.$$

Now we prove that the function $T_1(\beta)$ satisfies the hypotheses of Theorem 1 (of course such a proof can be extended to all $t \neq 1$ by only varying the index α of the summation method).

The Nth remainder of $T_1(\beta)$ is given by

$$R_N(\beta) \equiv T_1(\beta) - \sum_{k=0}^{N-1} a_k \beta^k = \int_{-\infty}^{+\infty} (2\pi)^{-1/2} e^{-x^2} \times ((-\beta)^N / N!) x^{N(m+1)} e^{Nx} e^{-\eta\beta x^{m+1} e^x}\, dx, \quad (23)$$

where $0 \leqslant \eta \leqslant 1$, $\eta = \eta(\beta x^{m+1} e^x)$, and $\Sigma_k a_k \beta^k$ is the asymptotic series expansion of $T_1(\beta)$. $R_N(\beta)$ is obviously analytic on the whole Riemann surface of the logarithm (e.g., by the translation $x \to x - \ln\beta$). Let $\theta \equiv \arg(\beta) \geqslant 0$. Then we distinguish between the cases $\theta \leqslant cm$ and $\theta > cm$, with fixed $c \gg 1$. If $\theta \leqslant cm$, by using the translation $x \to x - i\theta$, it is not difficult to obtain the required bound (2) for the behavior with respect to N.

If $\theta > cm$ let us choose the path

$$x \equiv x(y) = y - i\theta + i\epsilon - (m+1)\ln(y - i\theta), \quad y \in \mathbb{R} \quad (24)$$

for fixed ϵ in $(0,\pi/2)$. Then $dx = (1 - (m+1)(y - i\theta)^{-1})dy$, whence $|dx| \leqslant C_1\, dy$. Moreover $|\exp\{-\eta\beta(x(y))^m e^{x(y)}\}| \leqslant 1$. Let us fix $\gamma \ll (m+1)^{-1}$; then, for $y \in (-\infty, \gamma\theta)$ we have

$$|e^{-x^2}| \leqslant \exp(-(y - (m+1)\ln|y - i\theta|)^2) \times \exp((-\theta + \epsilon_0 + (m+1)\pi/2)^2) \quad (25)$$

for some $\epsilon_0 > 0$. Therefore,

$$|R_N(\beta)| \leqslant (|\beta|^N/N!) C_1 \int_{-\infty}^{\gamma\theta} \exp((-\theta + \epsilon_0 + (m+1)\pi/2)^2 + o(\theta)) e^{-(y - (m+1)\ln|y|)^2} \times |y - (m+1)\ln|y||^{(m+1)N} e^{Ny - (m+1)N\ln|y|}\, dy + (|\beta|^N/N!) C_1 \int_{\gamma\theta}^{+\infty} \exp(-(y - (m+1) \times \ln|y|)^2) e^{\theta^2 + o(\theta)} |y - (m+1) \times \ln|y||^{(m+1)N} e^{Ny} |y|^{-(m+1)N}\, dy. \quad (26)$$

The first integral in (26), by the inequality

$$|y - (m+1)\ln|y||^{(m+1)N} \leqslant (mN + N + 1) 2^{(m+1)N} \{|y|^{(m+1)N} + ((m+1)\ln|y|)^{(m+1)N}\}$$

and by a saddle point argument,[14] turns out to be less than $(C_2)^N (|\beta|^N/N!) \times \exp((-\theta + \epsilon_1 + (m+1)\pi/2)^2) N^{(m+1)N} e^{N^2/4}$ (27)

for some C_2, $\epsilon_1 > 0$.

In order to estimate the second integral in (26) let us distinguish the cases $N \geqslant 2\gamma^2\theta$ and $N < 2\gamma^2\theta$.

If $N \geqslant 2\gamma^2\theta$ the second integral, in analogy with (27), is bounded by

$$(C_3)^N \exp((-N/2\gamma^2)(2\epsilon + (m+1)\pi)) \times (|\beta|^N/N!)e^{\theta^2 + o(\theta)}N^{(m+1)N}e^{N^2/4} \leqslant (C_4)^N |\beta|^N e^{\theta^2 + o(\theta)}e^{-(2\epsilon + (m+1)\pi)\theta}(mN)!e^{N^2/4}. \quad (28)$$

If $N < 2\gamma^2\theta$ the integrand is nonincreasing in the interval $(\gamma\theta, +\infty)$ (provided that $\gamma \ll (m+1)^{-1}$) and the second integral in (26) is bounded by

$$(C_5)^N(|\beta|^N/N!)e^{\theta^2 + o(\theta)} \exp(-(\gamma\theta - (m+1)\ln(\gamma\theta))^2) \times \{(\gamma\theta)^{(m+1)N} + ((m+1)\ln(\gamma\theta))^{(m+1)N}\}e^{N\gamma\theta} \leqslant C_6(C_5)^N(|\beta|^N/N!)\exp((\theta - \epsilon_1 - (m+1)\pi/2)^2), \quad (29)$$

since $e^{-\gamma^2\theta^2 + N\gamma\theta} \leqslant e^{-\theta^2(\gamma^2 - 2\gamma^3)}$, where γ is small.

Therefore, by combining (27), (28), (29), and the analogous estimate for $\theta \leqslant cm$, we have

$$|R_N(\beta)| \leqslant A_0 \exp((-\theta + \epsilon_1 + (m+1)\pi/2)^2)(mN)! \times e^{N^2/4}(\delta_0)^N|\beta|^N \quad (30)$$

uniformly for $N \in \mathbb{N}$ and $\theta \geqslant 0$. In a similar way one can proceed for $\theta < 0$. Thus the hypothesis of Theorem 1 is verified and $T_1(\beta)$ is uniquely defined by the asymptotic series $\Sigma_k a_k \beta^k$ through the generalized Borel sum of order $(1,m)$ as defined in the present work.

APPENDIX: PROOF OF THE ASYMPTOTIC BEHAVIORS (5) AND (6)

Let $t_0 = t_0(w)$ be the solution of the equation $t^{-2} - 2\alpha^{-1}t^{-1}\ln(wt) = 0$ defined for $w > 0$ and analytically continued on the Riemann surface of $\ln w$, for $|w|$ large. In any finite sector of this surface we have

$$t_0(w) = \left(\frac{\alpha}{2}\right)\left(\ln\frac{w\alpha}{2}\right)^{-1} \times \left(1 + O\left(\left(\ln\ln\frac{w\alpha}{2}\right)\left(\ln\frac{w\alpha}{2}\right)^{-1}\right)\right) \quad \text{as } w \to \infty. \quad (A1)$$

By the substitution $t = t_0(w)\tau$ in (3) we have

$$\rho(w) = (\pi\alpha)^{-1/2}(wt_0)^{-1}e^{-\alpha^{-1}(\ln(wt_0))^2} \times \int_0^\infty \exp(-2\alpha^{-1}(\ln(wt_0))\,p(\tau))\,q(\tau)d\tau, \quad (A2)$$

where $p(\tau) = \tau^{-1} + \ln\tau$, $q(\tau) = e^{\alpha^{-1}(\ln\tau)^2}\tau^{-2}$, and the integral in (A2) is uniformly convergent for $\mathrm{Re}\ln(wt_0) > 0$. Since $p'(\tau) = 0$ for $\tau = 1$, an application of the Laplace method (Ref. 14, Chap. 4, Theorem 7.1) yields the asymptotic behavior as $wt_0 \to \infty$ in any finite sector of the Riemann surface of $\ln(wt_0)$

$$\rho(w) \sim (\pi/\alpha)^{-1/2}\Gamma(\tfrac{1}{2})(wt_0)^{-1} \times \exp(-\alpha^{-1}((\ln wt_0)^2 + \ln wt_0))(\alpha^{-1}\ln wt_0)^{-1/2}. \quad (A3)$$

Inserting (A1) in (A3) we obtain (5).

By an analogous substitution in the integral (4) and by choosing a contour $\gamma(1,\epsilon)$ containing the saddle point $\tau = 1$[14] we have

$$\sigma(w) \sim (\alpha/\pi)^{1/2}\Gamma(\tfrac{1}{2}) \times \exp(\alpha^{-1}(\ln wt_0)^2 + 2\ln wt_0)(\alpha^{-1}\ln wt_0)^{-1/2} \quad (A4)$$

in the same limit of (A3), whence (6) follows.

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On the solutions to a class of nonlinear integral equations arising in transport theory

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(Received 9 March 1984; accepted for publication 1 June 1984)

Existence and uniqueness for the solutions to a class of nonlinear equations arising in transport theory are investigated in terms of a real parameter α which can take on positive and negative values. On the basis of contraction mapping and positivity properties of the relevant nonlinear operator, iteration schemes are proposed, and their convergence, either pointwise or in norm, is studied.

PACS numbers: 02.30.Rz, 05.60. + w

I. INTRODUCTION

In this paper we shall consider the problem of solving the nonlinear integral equation

$$h(x) + \alpha h(x) \int_a^b K(x,y) h(y)\, dy = S(x), \quad x \in (a,b), \tag{1}$$

where $K(x,y)$ and $S(x)$ are real non-negative functions in the real domains $(a,b)\times(a,b)$ and (a,b), respectively, and α is a real parameter. The class of nonlinear integral equations described in Eq. (1) includes the nonlinear particle transport equation when removal effects are dominant.[1,2] In that case the dependent variable x is the particle speed ranging from 0 to ∞, α is equal to unity, the known term $S(x)$ is the intensity of the external source, the unknown $h(x)$ is related to the particle distribution function $f(x)$ by

$$h(x) = G(x) f(x),$$

where G is the positive macroscopic removal collision frequency of the host medium, and finally the (symmetric) kernel $K(x,y)$ is given by

$$K(x,y) = \frac{1}{2xG(x)G(y)} \int_{|x-y|}^{x+y} u g(u)\, du,$$

where g is the microscopic removal collision frequency by the particles between themselves. On the other hand, Eq. (1) is also a generalization of a famous equation in transport theory, the so-called Chandrasekhar H-equation[3,4] in which x ranges from 0 to 1, $\alpha = -1$, $S(x) = 1$, h must be identified with the H-function, and

$$K(x,y) = x\psi(y)/(x+y)$$

for a non-negative characteristic function ψ. This latter equation has been widely studied in the literature,[5,6] and due to the analyticity properties of its kernel, it has been possible to determine exactly the number and properties of solutions, and even to write them out explicitly.

In this paper, after a preliminary investigation based on contraction mapping, we shall mainly employ positivity arguments to study the existence and uniqueness of solutions to Eq. (1), with particular emphasis on positive solutions, that for the applications mentioned before, are the only physical ones. The convergence of iterative schemes for the solution of Eq. (1) will also be demonstrated.

Throughout this paper we shall assume that $S \in L_p(a,b)$ for some p, with $1 \leqslant p \leqslant \infty$, and that the linear integral operator

$$(Tf)(x) = \int_a^b K(x,y) f(y)\, dy \tag{2}$$

is a bounded mapping of $L_p(a,b)$ into $L_\infty(a,b)$, with norm $\|T\|$. A sufficient condition for that would be[7]

$$\operatorname*{ess\,sup}_{x\in(a,b)} \int_a^b |K(x,y)|^q\, dy = M < \infty, \quad \frac{1}{p} + \frac{1}{q} = 1, \tag{3}$$

in which case $\|T\| \leqslant M^{1/q}$. Further conditions that will be needed in some occasions are the following.

Assumption 1: The function S is continuous and the kernel K satisfies the requirement

$$\lim_{x_1 \to x_2} \int_a^b |K(x_1,y) - K(x_2,y)|^q\, dy = 0, \quad x_1, x_2 \in (a,b) \tag{4}$$

for any $y \in (a,b)$.

Assumption 2: $(TS)(x)$ is bounded away from zero, namely,

$$\operatorname*{ess\,inf}_{x\in(a,b)} \int_a^b K(x,y) S(y)\, dy = \delta > 0. \tag{5}$$

We note that Eq. (1) may be rewritten either as

$$h = A(h), \quad A(h) = S - \alpha h\, Th, \tag{6a}$$

or as

$$h = B(h), \quad B(h) = S/(1 + \alpha Th), \tag{6b}$$

both operators A and B being nonlinear, with $A(0) = B(0) = S$.

Equations (1) can also be regarded as a particular Hammerstein equation; for example setting

$$h(x) = [1 + \alpha f(x)]^{-1} \tag{7}$$

one ends up with the equation of Hammerstein type[8]

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$$f(x)=\int_a^b K(x,y)\,\phi\,[\,y,f(y)]\,dy,\quad \phi(x,u)=\frac{1}{(1+\alpha u)},$$

where however the usual assumption of continuity of ϕ with respect to u is violated at $u=-1/\alpha$.

II. GENERAL RESULTS

We can obtain some quite general results by applying the contraction mapping theorem to the operator A in Eq. (6a). If h belongs to the closed ball of L_p with center at the origin and radius r, namely $\|h\|\leqslant r$, we get at once

$$|A(h)|\leqslant S+|\alpha|\,|h|\,|Th|\leqslant S+|\alpha|\,\|T\|\,\|h\|\,|h|$$

and then

$$\|A(h)\|\leqslant\|S\|+|\alpha|\,\|T\|\,\|h\|^2\leqslant\|S\|+|\alpha|\,\|T\|r^2.$$

In order to insure that $\|A(h)\|\leqslant r$ we impose

$$|\alpha|\,\|T\|r^2-r+\|S\|\leqslant 0,$$

which leads to the conditions

$$|\alpha|\leqslant 1/(4\|T\|\,\|S\|) \tag{8}$$

and

$$\frac{1-\sqrt{1-4|\alpha|\,\|T\|\,\|S\|}}{2|\alpha|\,\|T\|}\leqslant r\leqslant\frac{1+\sqrt{1-4|\alpha|\,\|T\|\,\|S\|}}{2|\alpha|\,\|T\|}. \tag{9a}$$

Further, for A to be a contraction, we note that

$$\begin{aligned}|A(h_1)-A(h_2)|&=|\alpha|\,|h_2(Th_2-Th_1)+(h_2-h_1)\,Th_1|\\&\leqslant|\alpha|(\|T\|\,\|h_2-h_1\|\,|h_2|\\&\quad+\|T\|\,\|h_1\|\,|h_2-h_1|)\end{aligned}$$

so that

$$\begin{aligned}\|A(h_1)-A(h_2)\|&\leqslant|\alpha|\,\|T\|(\|h_2\|+\|h_1\|)\|h_1-h_2\|\\&\leqslant 2r|\alpha|\,\|T\|\,\|h_1-h_2\|,\end{aligned}$$

which leads to the restriction

$$r<1/(2|\alpha|\,\|T\|). \tag{9b}$$

We can then state[9] the following.

Theorem 1: If α satisfies Eq. (8), there exists a unique solution h^* to Eq. (1) in any closed ball of $L_p(a,b)$ centered at the origin with radius r such that

$$\frac{1-\sqrt{1-4|\alpha|\,\|T\|\,\|S\|}}{2|\alpha|\,\|T\|}\leqslant r\leqslant\frac{1}{2|\alpha|\,\|T\|}. \tag{10}$$

Moreover, the iteration scheme

$$h_n=A(h_{n-1}) \tag{11}$$

converges in the L_p-norm to this unique solution if the initial guess h_0 is chosen in the ball.

This theorem is valid under the general hypotheses of the Introduction [$S(x)$ and $K(x,y)$ non-negative, $S\in L_p$, T is a bounded operator of L_p into L_∞]. In this theorem, however, the non-negativity of S and K plays no role, and can be dropped.

A trivial corollary of the theorem is

$$\|h^*\|\leqslant\frac{1-\sqrt{1-4|\alpha|\,\|T\|\,\|S\|}}{2|\alpha|\,\|T\|} \tag{12}$$

and that other solutions, if any, will have a norm not less than $1/(2|\alpha|\,\|T\|)$.

If now, in addition to non-negativity of S and K, we assume that α is positive, we can sharpen Theorem 1 to show the following.

Theorem 2: Let $\alpha>0$ satisfy Eq. (8). Then Eq. (1) has at least one non-negative solution $h^*\in L_p$ with

$$\frac{\sqrt{1+4\alpha\|T\|\,\|S\|}-1}{2\alpha\|T\|}\leqslant\|h^*\|\leqslant\|S\|, \tag{13}$$

which is the unique L_p-solution with norm less than $1/(2\alpha\|T\|)$, and is the limit (in the L_p-norm) of the iterative scheme (11) for any initial guess h_0 with

$$\|h_0\|\leqslant\frac{1-\sqrt{1-4\alpha\|T\|\,\|S\|}}{2\alpha\|T\|}. \tag{14}$$

If in addition h_0 is non-negative and less than S, all h_n are also non-negative and less than S. [Whenever the context is clear, we will use the notation $g\leqslant f$ to mean $g(x)\leqslant f(x)$ a.e. for $x\in(a,b)$.]

Proof: The proof of this last theorem follows quickly from Theorem 1. The unique solution h^* in the ball defined by Eq. (10) is the limit of the sequence (11), and is independent of h_0, provided h_0 satisfies Eq. (14). We then take $0\leqslant h_0\leqslant S$, and show by induction that $0\leqslant h_n\leqslant S$. Suppose $0\leqslant h_{n-1}\leqslant S$; then $h_n\leqslant S$ follows immediately from Eq. (6a) for $\alpha>0$ and $h_{n-1}\geqslant 0$. In addition,

$$\begin{aligned}h_n=A(h_{n-1})&\geqslant S[\,1-\alpha Th_{n-1}\,]\\&\geqslant S[\,1-\alpha\|T\|\,\|h_{n-1}\|\,]\geqslant 0,\end{aligned}$$

since $\|h_{n-1}\|<1/(\alpha\|T\|)$ is guaranteed *a fortiori*, h_{n-1} being in the ball (10). This proves both inequalities for h_n, and thus for h^* in the limit for $n\to\infty$. Therefore, $0\leqslant h^*\leqslant S$, and $\|h^*\|\leqslant\|S\|$ [which is of course stronger than Eq. (12)]. Finally, we note from Eq. (1) with $\alpha>0$ and $h^*\geqslant 0$ that

$$\|S\|\leqslant\|h^*\|+\alpha\|h^*\|\,\|Th^*\|\leqslant\|h^*\|+\alpha\|T\|\,\|h^*\|^2$$

from which the other inequality in Eq. (13) follows directly. This completes the proof of the theorem.

From this proof we also note further that starting from a non-negative initial guess in the ball $\|h\|\leqslant\|S\|$ the iterative procedure is positivity preserving inside the same ball for

$$\alpha<1/(\|T\|\,\|S\|), \tag{15}$$

which is weaker than the condition for convergence given by Eq. (8).

There of course may be other solutions of Eq. (1) than h^*. In this regard we write

Lemma 1: Let $\alpha>0$, and suppose that a nonpositive solution $\hat{h}$ to Eq. (1) exists in L_p. Then

$$\|\hat{h}\|\geqslant\frac{1+\sqrt{1+4\alpha\|T\|\,\|S\|}}{2\alpha\|T\|}. \tag{16}$$

[Note that the right-hand side is greater than $1/(\alpha\|T\|)$ which is twice the lower bound in Theorem 1.]

Proof: To prove Eq. (16) it is sufficient to write $S=-\hat{h}[\alpha T(-\hat{h})-1]$, with S and $-\hat{h}$ non-negative, and $\alpha[T(-\hat{h})]>1$, so that, taking norms, we find

$$\begin{aligned}\|S\|&\leqslant\|\hat{h}\|\ \text{ess sup}[\alpha T(-\hat{h})-1]\leqslant\|\hat{h}\|(\alpha\|T\|\,\|\hat{h}\|-1)\\&=\alpha\|T\|\,\|\hat{h}\|^2-\|\hat{h}\|,\end{aligned}$$

which yields

$$\alpha\|T\|\,\|\hat{h}\|^2-\|\hat{h}\|-\|S\|\geqslant 0$$

from which Eq. (16) easily follows.

Another general result can be established for positive α. We write

Lemma 2: Let $\alpha > 0$ and Assumption 1 hold. Then, if a non-negative solution $h \in L_p$ exists, this solution is necessarily continuous, and is positive if and only if S is positive.

Proof: By Eq. (4) T maps L_p functions into continuous functions, so that $1 + \alpha Th$ is continuous and bounded away from zero. Thus $B(h)$ is continuous since S is continuous and vanishes where S is zero, and only there.

We can complete Theorem 2 and Lemma 1 by writing

Theorem 3: If a solution h to Eq. (1) exists, and there exists an $\epsilon > 0$ for which

$$\|h\| \leqslant (1-\epsilon)/|\alpha|\,\|T\|, \tag{17}$$

then h is non-negative. It is also continuous when Assumption 1 holds.

Proof: The proof follows from $1 + \alpha Th > \epsilon$, which ensures that the denominator of $B(h)$ is positive and bounded away from zero (and continuous under Assumption 1).

Results somewhat similar to Theorems 2 and 3 can also be shown for the case $\alpha < 0$. It proves convenient to refer to Eq. (6a), and look for the fixed points of the operator A defined by

$$A(h) = S + \beta hTh, \quad \beta = -\alpha = |\alpha| > 0. \tag{18}$$

It is clear that now A has several nice properties. It is a continuous operator in L_p, since from

$$\begin{aligned} |A(f_1) - A(f_2)| &= \beta\,|(f_1 - f_2)\,Tf_1 + f_2T(f_1 - f_2)| \\ &\leqslant \beta\,\|T\|(\|f_1\|\,|f_1 - f_2| + \|f_1 - f_2\|\,|f_2|) \end{aligned}$$

it is easily seen that for any $f_1, f_2 \in L_p$,

$$\|A(f_1) - A(f_2)\| \leqslant \beta\,\|T\|(\|f_1\| + \|f_2\|)\|f_1 - f_2\|. \tag{19}$$

In addition, A is positive [$f \geqslant 0$ implies $A(f) \geqslant S \geqslant 0$] and monotone in the cone of the non-negative functions, since for $f_1 \geqslant f_2$ we have

$$A(f_1) - A(f_2) = \beta(f_1 - f_2)\,Tf_1 + \beta f_2T(f_1 - f_2) \geqslant 0. \tag{20}$$

We can prove

Lemma 3: Let $\beta = -\alpha > 0$ and

$$\beta \leqslant 1/(4\|T\|\,\|S\|). \tag{21}$$

Then the operator A maps the so-called conical segment[10] $\langle 0, cS\rangle$ into itself for any c such that

$$\frac{1 - \sqrt{1 - 4\beta\|T\|\,\|S\|}}{2\beta\|T\|\,\|S\|} \leqslant c \leqslant \frac{1 + \sqrt{1 - 4\beta\|T\|\,\|S\|}}{2\beta\|T\|\,\|S\|}. \tag{22}$$

Proof: If in fact h belongs to the conical segment $\langle 0, cS\rangle$ we get

$$A(h) \geqslant S \geqslant 0$$

and

$$A(h) = S + \beta hTh \leqslant S + \beta c^2 STS \leqslant S + \beta c^2 \|T\|\,\|S\|S.$$

Thus the requirement $A(h) \leqslant cS$ leads to the inequality

$$\beta\,\|T\|\,\|S\|c^2 - c + 1 \leqslant 0,$$

which is equivalent to Eqs. (21) and (22). Note that the left-hand side in Eq. (22) is always greater than unity.

From the continuity and monotonicity of A, from Lemma 3, and from the regularity of the cone of the non-negative functions in L_p, we can deduce immediately[10] the following.

Theorem 4: Under the assumptions of Lemma 3, Eq. (6a) has at least one non-negative solution h^* belonging to the conical segment $\langle 0, cS\rangle$, where c satisfies Eq. (22), and which is given by the limit (pointwise and in norm) of the monotonic successive approximations

$$h_{n+1} = A(h_n), \quad h_0 = S. \tag{23}$$

The conical segment to which h^* belongs can further be sharpened by observing that for any non-negative solution we have $h = A(h) \geqslant S$, so that we may write

$$S \leqslant h^* \leqslant \frac{1 - \sqrt{1 - 4\beta\|T\|\,\|S\|}}{2\beta\|T\|\,\|S\|}\,S. \tag{24}$$

It is worth noticing that Theorem 4 and Eq. (24) are in agreement with Theorem 1 and Eq. (12), and that Eq. (8) coincides with Eq. (21). The results are complementary and strengthen each other. The solution h^* of both theorems can be obtained starting from any initial guess allowed by Theorem 1, the solution is non-negative and satisfies Eq. (24) (Theorem 4), and there are no other solutions with norm less than $1/(2\beta\|T\|)$ (Theorem 1). Other solutions, possibly positive, might occur beyond the latter limit. When β is larger than $1/(4\|T\|\,\|S\|)$, a non-negative solution might even fail to exist.

The results obtained so far all require restrictions on the parameter α. We might search for conditions ensuring the existence and possibly the uniqueness of non-negative solutions to Eq. (1) without restrictions on the parameter α. However, the simple examples in the following section illustrate that this search might be fruitless for the case $\alpha < 0$.

III. SOME EXAMPLES

Equation (1) can be reduced to the solution of a system of transcendental equations for a finite number of scalar coefficients when the kernel $K(x, y)$ is degenerate (of finite rank N), namely,

$$K(x, y) = \sum_{n=1}^{N} X_n(x) Y_n(y) \tag{25}$$

with for instance $Y_n \in L_p$, $X_n \in L_\infty$, and of course $X_n \geqslant 0$, $Y_n \geqslant 0$. We will consider two very simple examples with the lowest possible order of degeneracy.

Example 1: $K(x, y) = \text{const} = k$. Setting

$$\xi = \int_a^b h(x)\,dx, \quad s = \int_a^b S(x)\,dx$$

we get at once

$$h(x) = S(x)/(1 + \alpha k\xi). \tag{26}$$

Now integrating over x, we obtain the second-degree algebraic equation for ξ

$$\alpha k\xi^2 + \xi - s = 0, \tag{27}$$

which always has two roots, with different features according to the values of α, k, and s. For $\alpha > 0$ there are always two real solutions

$$\xi = (-1 \pm \sqrt{1 + 4\alpha ks})/2\alpha k, \tag{28}$$

one positive, with the lower magnitude, and one negative, in agreement with Eqs. (13) and (16), respectively, but without any other restriction on α. When $\alpha < 0$, and if we are interest-

ed in real solutions only, there are no solutions for $|\alpha| > 1/(4ks)$ [see Eq. (8)], and there are two positive roots for ξ when $|\alpha| < 1/(4ks)$. Thus for the original unknown $h(x)$ we obtain one non-negative and one nonpositive solution (the latter with larger norm) for $\alpha > 0$, two non-negative solutions for $-1(4ks) < \alpha < 0$, and no solutions for $\alpha < -1/(4ks)$. In this example the solution is in fact reduced to the analysis of a quadratic algebraic equation and the solution depends merely on the sign of the numerical coefficients. Note that the factor $1 + \alpha k\xi$ never vanishes.

It seems reasonable to expect similar trends in general for Eq. (1). Of course the similarity cannot be interpreted literally, as shown by the following example.

Example 2: $h(x) + xh(x)\int_0^1 yh(y)\,dy = 1$. Setting

$$\xi = \int_0^1 xh(x)\,dx$$

we get at once $(1 + \xi x)\,h(x) = 1$, and then

$$h(x) = 1/(1 + \xi x), \tag{29}$$

where for an L_p-solution we discard all values of ξ less than or equal to -1. For $\xi = 0$ we would get $h = 1$ which contradicts the hypothesis $\xi = 0$. For $-1 < \xi < 0$ or $\xi > 0$ we multiply Eq. (29) by x and integrate, to get

$$\xi = 1/\xi - (1/\xi^2)\ln|1 + \xi|. \tag{30}$$

For $\xi > -1$, $\xi \neq 0$ all the roots of the transcendental equation (not algebraic any more, so that the number of roots is unknown *a priroi*) yield a positive solution h in L_p. It is easy to check that there is only one root $\xi_0 \neq 0$, with $0 < \xi_0 < 1$. Thus as in Example 1 (with $\alpha > 0$), there is a unique non-negative solution, but now no other solutions exist, neither negative, nor of changing sign.

Other well-known examples are available in the literature. The Chandrasekhar H-equation

$$H(x) - xH(x)\int_0^1 \frac{\psi(y)}{x+y}\,h(y)\,dy = 1, \tag{31}$$

with

$$\psi(x) \geqslant 0, \quad \psi_0 = \int_0^1 \psi(x)\,dx \leqslant \frac{1}{2},$$

($\alpha = -1$ in our notation) has one solution which is positive on (0,1) for $\psi_0 = \frac{1}{2}$ and two positive solutions or just one positive solution for $\psi_0 < \frac{1}{2}$ depending on the particular form of $\psi(x)$.[5] In the former case the modified form of the same equation[4]

$$F(x) + \frac{F(x)}{\sqrt{1-2\psi_0}}\int_0^1 \frac{y\psi(y)F(y)}{x+y}dy = \frac{1}{\sqrt{1-2\psi_0}} \tag{32}$$

(with $\alpha > 0$ in our notation) has two solutions, one positive and one negative on (0,1), and no other solutions.[11]

Example 1 above shows the non-negative solutions can actually fail to exist for some negative values of the parameter α, and that for other negative values of α two non-negative solutions can also actually occur, even in the simplest case where Eq. (6a) is amenable to a simple quadratic algebraic equation. It is then apparent that in general (i.e., without restrictions on α) existence and/or uniqueness theorems can not be formulated. However, for $\alpha > 0$ some very general results independent of the magnitude of α can be formulated. These results require only the very weak conditions on S and K outlined in the Introduction.

IV. THE CASE OF POSITIVE α

In this section we will look for non-negative solutions to Eq. (1) when $\alpha > 0$. In particular we look for non-negative fixed points of the operator B in Eq. (6b), which is more convenient to handle than A, since it is always positivity preserving. It is clear that the linear operator T is positive ($f \geqslant 0$ implies $Tf \geqslant 0$) and monotone[10] ($f_1 \geqslant f_2$ implies $Tf_1 \geqslant Tf_2$). B is also positive, but not montone, since $f_1 \geqslant f_2$ implies $B(f_1) \leqslant B(f_2)$. But just for this reason B^2 (still positive) is then monotone, i.e., $B^2(f_1) \geqslant B^2(f_2)$. Other properties of B with respect to the cone of the non-negative functions in L_p are $B(f) \leqslant S$ and $B(f) \geqslant S/(1 + \alpha\|T\|\,\|f\|)$ for $f \geqslant 0$, namely

$$\alpha_1(f)S \leqslant B(f) \leqslant \beta_1(f)S, \quad \alpha_1(f) = [1 + \alpha\|T\|\,\|F\|]^{-1},$$
$$\beta_1(f) = 1, \tag{33}$$

for any $f \geqslant 0$. Also, for any $f \geqslant 0$ and $\gamma \in (0,1)$ we have

$$\frac{B(\gamma f)}{B(f)} = \frac{1 + \alpha Tf}{1 + \gamma\alpha Tf} = 1 + (1-\gamma)\frac{\alpha Tf}{1 + \gamma\alpha Tf} \geqslant 1 = \gamma + (1-\gamma),$$
$$1 - \gamma = \eta > 0. \tag{34}$$

Equations (33) and (34) guarantee that B is S-concave.[10]

Moreover B is a continouous operator with respect to the cone of non-negative functions in L_p. We have in fact, for $f_1, f_2 \in L_p(a,b)$, f_1 and f_2 non-negative, $\alpha > 0$

$$|B(f_1) - B(f_2)| = \frac{\alpha S\,|Tf_2 - Tf_1|}{(1 + \alpha Tf_1)(1 + \alpha Tf_2)} \leqslant \alpha\|T\|\,\|f_1 - f_2\|S$$

and thus

$$\|B(f_1) - B(f_2)\| \leqslant \alpha\|T\|\,\|S\|\,\|f_1 - f_2\|, \tag{35}$$

which proves the continuity, and shows that Eq. (15) above is a condition for B to be a contraction.

As for the problem of non-negative solution to Eq. (6b), we remark that if h is such a solution, then $h \leqslant S$ and $h = B(h) \geqslant B(S)$. All non-negative solutions are then located in the strip.

$$\frac{S}{1 + \alpha\|T\|\,\|S\|} \leqslant \frac{S}{1 + \alpha TS} \leqslant h \leqslant S. \tag{36}$$

With these results at hand we can now draw the following conclusions.

Lemma 4: Let $\alpha > 0$. Consider the successive approximation scheme

$$h_n = B(h_{n-1}), \quad h_0 = 0, \tag{37}$$

where obviously $0 \leqslant h_n \leqslant S$. Then (i) the even subsequence $\{h_n\}, n = 0, 2, 4, \ldots$, is monotonically nondecreasing and converges pointwise and in norm to a non-negative limit $h^e \leqslant S$ belonging to L_p; (ii) the odd subsequence $\{h_n\}, n = 1, 3, 5, \ldots$, is monotonically nonincreasing and converges point-wise and in norm to a non-negative limit $h^o \leqslant S$ belonging to L_p; (iii) any approximation from the even subsequence is less than or equal to any approximation from the odd subsequence (no overlapping); and finally (iv) the even and odd limits are such that

$$h^e \leqslant h^0, \quad h^0 - h^e = \alpha(h^e T h^o - h^o T h^e). \tag{38}$$

Proof: Note first that if $h_{n-1} \leqslant h_n$, then $B(h_{n-1}) \geqslant B(h_n)$. Thus we have $h_n \geqslant h_{n+1}$, $h_{n+1} \leqslant h_{n+2}$, and so on (reversed at any step). Now if $h_{n-1} \leqslant h_{n+1}$, then by analogous argument we see that $h_n \geqslant h_{n+2}$, $h_{n+1} \leqslant h_{n+3}$, and so on (conserved for terms of the same parity). Because we have taken $h_0 = 0$, we have $h_0 \leqslant h_1 = S$ and $h_0 \leqslant h_2 = S[1 + \alpha TS]^{-1}$. Thus the oscillating behavior of the sequence, the monotonicity of subsequences, and the non-overlapping follow by induction. Because the subsequences are bounded above and below by S and 0, respectively, they converge pointwise. Further because the cone of non-negative functions in L_p is regular,[10] the even and odd subsequences also converge in L_p norm to $h^e \in L_p$ and $h^o \in L_p$, respectively, both limits lying in the strip (36). If $h^e = h^0$, Eq. (38) is obviously true. If $h^e \neq h^o$ the two limits must be related by

$$h^e = \frac{S}{1 + \alpha T h^0} = B(h^0), \quad h^0 = \frac{S}{1 + \alpha T h^e} = B(h^e) \tag{39}$$

from which Eq. (38) follows.

Sufficient conditions for the convergence of the iterative scheme (37) are given by the following.

Lemma 5: Let $\alpha > 0$ and suppose that either Eq. (15) holds or the kernel K is symmeric, i.e., $K(y,x) = K(x,y)$. Then

$$\begin{aligned} |h_{n+1} - h_{n-p+1}| &= \left| B\left(\frac{1}{n}\sum_{j=1}^{n} h_j\right) - B\left(\frac{1}{n-p}\sum_{j=1}^{n-p} h_j\right)\right| \\ &\leqslant \alpha S \left| \left(\frac{1}{n-p} - \frac{1}{n}\right)\sum_{j=1}^{n-p} Th_j - \frac{1}{n}\sum_{j=n-p+1}^{n} Th_j \right| \\ &\leqslant \alpha \|T\| S \left[\frac{p}{n(n-p)}\sum_{j=1}^{n-p} \|h_j\| + \frac{1}{n}\sum_{j=n-p+1}^{n} \|h_j\|\right] \\ &\leqslant 2\frac{p}{n}\alpha \|T\| \, \|S\| S. \end{aligned}$$

Thus for any fixed p we have (since $S \in L_p$)

$$\lim_{n\to\infty} |h_{n+1} - h_{n-p+1}| = 0 = \lim_{n\to\infty} \|h_{n+1} - h_{n-p+1}\|$$

so that a pointwise and L_p-limit h^* exist, and is in the strip (36). We now show that

$$\lim_{n\to\infty} \frac{1}{n}\sum_{j=1}^{n} h_j = h^* \tag{41}$$

in the sense of both pointwise and L_p-convergence. Let $\epsilon > 0$ be fixed, and n_ϵ be the corresponding index for which $|h^* - h_j| < \epsilon$ for any $j > n_\epsilon$. We may then write for $n > n_\epsilon$

$$\begin{aligned} \left|\frac{1}{n}\sum_{j=1}^{n} h_j - h^*\right| &\leqslant \frac{1}{n}\sum_{j=1}^{n_\epsilon} (|h^*| + |h_j|) \\ &\quad + \frac{1}{n}\sum_{j=n_\epsilon+1}^{n} |h^* - h_j| \\ &\leqslant 2\frac{n_\epsilon}{n} S + \left(1 - \frac{n_\epsilon}{n}\right)\epsilon \end{aligned}$$

and therefore the left-hand side can be made smaller than any fixed positive number, provided n is large enough. This proves Eq. (41) for the pointwise convergence. The proof of convergence in the L_p-norm proceeds in a similar manner with moduli replaced by norms. (It is understood, here and elsewhere that pointwise properties are "almost everywhere"; thus S could even diverge on a set of zero measure.) Note from Eq. (41) that the nth approximation is, when n is large, just the arithmetic average of the preceding ones. Now from Eq. (40) and the continuity of B it follows that $h^* = B(h^*)$, and the existence theorem is complete. We note in passing that the pointwise convergence $B((1/n)\Sigma_{j=1}^{n} h_j)$ to $B(h^*)$ can be proved even without continuity of B if we assume that T maps sequences in L_p converging in norm into pointwise converging sequences.

We now consider the problem of uniqueness of non-negative solutions. To this end note the following.

Lemma 6: Let $\alpha > 0$ and Assumption 2 hold. Then B^2 is an S-concave operator.[10]

Proof: From Eq. (33) we get directly, for any $h \in L_p$, $h \geqslant 0$

the even and odd limits of Lemma 4 coincide, and the common value h^* is a non-negative solution of Eq. (6b).

Proof: If Eq. (15) holds then the operator B is a contraction. If then $h^e \neq h^o$ we see from Eq. (39) that the contradiction

$$\|h^o - h^e\| = \|B(h^e) - B(h^o)\| < \|h^e - h^o\|$$

would follow. On the other hand, if the kernel K is symmetric, integration of Eq. (38) over (a,b) gives at once

$$\int_a^b [h^0(x) - h^e(x)]\, dx = 0,$$

where the integrand is non-negative. Thus we have $h^o = h^e = h^*$ and from Eq. (39) it follows finally that $h^* = B(h^*)$ which completes the proof.

Stronger results follow from the next theorem which gives the main result concerning existence of non-negative solutions.

Theorem 5: Let $\alpha > 0$, and consider the iterative scheme

$$h_{n+1} = B\left(\frac{1}{n}\sum_{j=1}^{n} h_j\right), \quad 0 \leqslant h_1 \leqslant S. \tag{40}$$

Then the sequence h_n converges pointwise and in the L_p-norm to a limit h^* in the strip (36) which is a non-negative solution of Eq. (6b).

Proof: All h_n, starting from h_2, are in the strip (36). For any fixed n, and p with $1 \leqslant p < n$ we have

$$\alpha_2(h)S \leqslant B^2(h) \leqslant \beta_2(h)S, \quad \alpha_2(h) = \alpha_1[B(h)],$$
$$\beta_2(h) = \beta_1[B(h)]. \tag{42}$$

We then consider, for a fixed non-negative h in L_p, and for a fixed γ with $0 < \gamma < 1$, the quantity $B^2(\gamma h)$; it can be shown that there exists a number $\eta = \eta(\gamma, h) > 0$ such that

$$B^2(\gamma h) \geqslant (1+\eta)\gamma B^2(h) \tag{43}$$

and therefore, by Eqs. (42) and (43), B^2 is S-concave. Proving Eq. (43) is equivalent to proving

$$1 + \alpha TB(h) \geqslant (1+\eta)\gamma[1 + \alpha TB(\gamma h)],$$

which is satisfied if

$$0 < \eta \leqslant \frac{1 - \gamma + \alpha T[B(h) - \gamma B(\gamma h)]}{\gamma[1 + \alpha TB(\gamma h)]}.$$

It is then sufficient to choose (since T is linear and positive)

$$0 < \eta \leqslant \frac{1-\gamma}{\gamma} \frac{\alpha}{1 + \alpha\|T\|\,\|S\|} \frac{\alpha_1(\gamma h)}{1 + \alpha\|T\|\,\|h\|} TS$$
$$\leqslant \frac{1-\gamma}{\gamma} \frac{\alpha}{1 + \alpha\|T\|\,\|h\|} \frac{TB(\gamma h)}{1 + \alpha TB(\gamma h)}$$

or by Eq. (5)

$$0 < \eta \leqslant \frac{1-\gamma}{\gamma} \frac{\delta}{1 + \alpha\|T\|\,\|S\|} \frac{\alpha_1(\gamma h)}{1 + \alpha\|T\|\,\|h\|}, \tag{44}$$

where the right-hand side is positive by Assumption 2.

Our final theorem gives sufficient conditions for uniqueness of non-negative solutions.

Theorem 6: Let $\alpha > 0$ and suppose either α satisfies Eq. (15) or Assumption 2 holds. Then Eq. (6b) has a unique non-negative solution h^* given by Theorem 5.

Proof: If Eq. (15) is satisfied, B is a contraction and h^* is necessarily the only non-negative solution, for if another non-negative solution $\hat{h}$ existed, with $\hat{h} \neq h^*$, we would immediately get the contradiction

$$\|h^* - \hat{h}\| = \|B(h^*) - B(\hat{h})\| < \|h^* - \hat{h}\|.$$

If Assumption 2 holds, then by the previous lemma, B^2 is S-concave, and as such it has at most one non-negative fixed point.[10] Since all fixed points of B are also fixed points of B^2, and one non-negative fixed point h^* of B exists, then h^* is necessarily the unique non-negative solution of Eq. (6b).

Corollary 1: Let the hypotheses of Theorem 6 be satisfied. Then the iterative scheme (40) converges to the same limit h^* whatever the initial guess h_1 in (40), and further the iterative scheme (37) also converges to h^* for any initial guess h_0, with $0 \leqslant h_0 \leqslant S$.

Proof: The first part of the corollary is a direct consequence of uniqueness. The second part follows from noting that the even subsequence is just the whole sequence for the equation $h = B^2(h)$ with initial guess h_0, and converges thus monotonically[10] to h^*, the unique non-negative fixed point of B^2 and B. The same occurs to add subsequence, which is the whole sequence for $h = B^2(h)$ with initial guess h_1.

V. CONCLUSIONS

We have given existence and uniqueness theorems for the solution of the nonlinear Eq. (1) under assumption of non-negativity and a couple of very mild smoothness requirements for the known term S and linear kernel K. Most of the theorems are constructive, since they provide the way to evaluate the solution. Particular emphasis has been given to the existence of non-negative solutions. For $\alpha > 0$ a non-negative solution always exists, and is unique under a very weak positivity assumption on K and S. In any case it is unique if α is small enough. On the other hand, for $\alpha < 0$ there is at least one non-negative solution as long as the magnitude of α is small enough, but it is in general not unique. Moreover, for $\alpha < 0$ and $|\alpha|$ large, non-negative solutions can fail to exist.

The analysis of bifurcation with respect to the parameter α deserves further investigation.

Another tool to get more insight into the problem would be a generalization of the analyticity argument used in Ref. 5 for the Chandrasekhar H-equation. It is always possible to rewrite Eq. (1) as

$$[h(x)]^{-1} = 1 + \alpha \int_a^b K(x,y)\, h(y)\, dy \tag{45}$$

and assuming that the new kernel satisfies

$$K(x,y)K(-x,z) = K(y,z)\,K(x,y) + K(z,y)\,K(-x,z), \tag{46}$$

one gets the factorization

$$[h(x)h(-x)]^{-1} = T(x)$$
$$\equiv 1 + \alpha \int_a^b [K(x,y) + K(-x,y)]\, dy, \tag{47}$$

which could allow some explicit results depending on the analyticity properties of the "dispersion function" $T(x)$. An example of a kernel satisfying Eq. (46) is provided by the straightforward generalization of Eq. (32)

$$K(x,y) = \frac{\phi(x)\psi(y)}{\phi(x) + \phi(y)} \tag{48}$$

with $\phi(-x) = -\phi(x)$, for which

$$T(x) = 1 + 2\alpha\phi^2(x) \int_a^b \frac{\psi(y)}{\phi^2(x) - \phi^2(y)}\, dy.$$

This approach will be, hopefully, a matter for further research.

ACKNOWLEDGMENTS

The authors would like to thank Professor J. Slawny for illuminating discussions. One of the authors (G.S.) wishes to thank the Laboratory for Transport Theory and Mathematical Physics, and the Physics Department at the Virginia Polytechnic Institute and State Univesity for their hospitality during the time this work was being carried out.

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Two theorems on star diagrams

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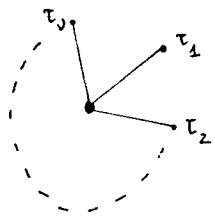
(Received 22 February 1984; accepted for publication 11 May 1984)

The notion of star diagram, previously introduced for the study of Green functions of nonlinear differential operators is formulated in an algebraic frame. Two theorems are presented which make the structure of these functions explicit.

PACS numbers: 02.30.Tb, 02.30.Hq

I. INTRODUCTION

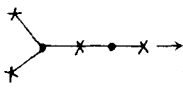
In preceding papers,[1,2] we introduced the notion of star diagrams, with the object of making the retarded n-point functions of some nonlinear differential operators explicit. A ν-star, $\nu = 0,1,2,...$,[3] is a diagram of the form



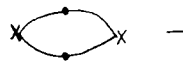
with which is associated the kernel

$$E_\nu(t;\tau_1,...,\tau_\nu) \equiv \theta(t - \sup(\tau_1,...,\tau_\nu))(\bar{\alpha}(t) - \bar{\alpha}(\sup(\tau_1,...,\tau_\nu))),$$

where $\bar{\alpha}$ is a given function. A star diagram is constituted by a juxtaposition of stars, tied by some of their extremities; in addition, to each of the extremities is assigned a cross that represents the source function η (vanishing for negative t). With such a diagram is associated the integral, over the variables τ, of the product of the kernels and source functions involved. For instance, we have the correspondences



$$\to \int d\tau_1\, d\tau_2\, d\tau_3\, d\tau_4\, \eta(\tau_1)\eta(\tau_2)\eta(\tau_3)\eta(\tau_4) \times E_3(t;\tau_1,\tau_2,\tau_3)\; E_2(t;\tau_3,\tau_4),$$



$$\to \int d\tau_1\, d\tau_2\, \eta(\tau_1)\eta(\tau_2)(E_2(t;\tau_1,\tau_2))^2.$$

In addition, an exceptional diagram represented by a single cross has to be introduced, with the correspondence rule

$$\times \to \bar{\eta}(t) \equiv \int_0^t d\tau\, \eta(\tau).$$

Disconnected diagrams may appear and the function associated with such a diagram is the product of the functions associated with each of its connected components.

The aim of the present paper is to prove the following theorems.

Theorem 1 : Let P be a polynomial with constant coefficients, α a given function, and η an arbitrary function of t, both continuous for $t \geqslant 0$ and vanishing for $t < 0$.[4] The retarded solution of the differential equation

$$\frac{dx}{dt} - \alpha(t)P(x) = \eta(t) \qquad \text{(E)}$$

is represented by a linear combination (generally infinite) of star diagrams, with $\bar{\alpha}(t) = \int_0^t \alpha(\tau)d\tau$.

Theorem 2 : Any star diagram is equivalent to a linear combination of tree star diagrams.

Theorem 1 allows us to give explicit algebraic expressions of the n-point functions G_n, the latter being defined as the kernels of the expansion of $x(t)$ considered as a functional of η, that is to say,

$$x(t) = \sum_{n=1}^{\infty} \frac{1}{n!} \int d\tau_1 \cdots d\tau_n\; G_n(t;\tau_1,...,\tau_n)\eta(\tau_1)\cdots\eta(\tau_n).$$

For instance, the kernels associated with the two preceding examples are, respectively,

$$4!\ \mathrm{sym}(E_3(t;\tau_1,\tau_2,\tau_3)\, E_2(t;\tau_3,\tau_4))$$

and

$$2!\ (E_2(t;\tau_1,\tau_2))^2,$$

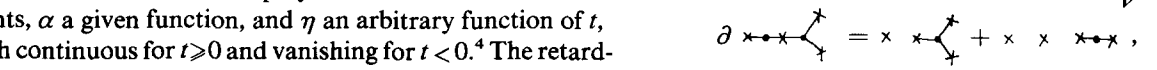
where sym means the symmetrization on the τ-variables. Afterwards, Theorem 2 asserts that $x(t)$ can be expressed exclusively with the help of trees.

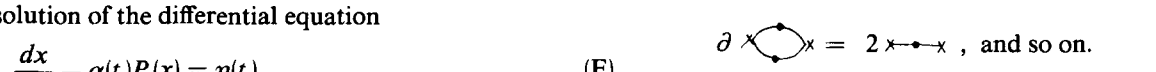
Thus the present results improve that of Ref. 2, in which stars of a more complicated structure appeared (stars with dressed centers), resulting in completely explicit expressions of the G_n's in the only case where P reduces to a monomial. In fact, they completely establish the conjecture put forward in Ref. 2.

II. PROOF OF THEOREM 1

In a first step, let us consider the star diagrams as abstract symbols (i.e., without reference to the value assigned to them in the Introduction). Let $\mathscr{A}$ be the free commutative algebra with unity generated by all the connected diagrams. In this algebra, the product of generators $A_1A_2 \cdots A_n$ is identified as the diagram having $A_1, A_2,...,A_n$ as connected components. Let ∂ be the derivation of $\mathscr{A}$ defined as follows: for any diagram A, the derivative ∂A is the sum of all possible diagrams obtained by removing from A one center of star. In particular,

$\partial \times = 0$, $\partial \bullet = 1$, ∂  $= \underbrace{\times \cdots \times}_{\nu}$,





It is obvious that $\mathscr{A}$ may be endowed with a structure of graded algebra, the degree of a diagram being the number N

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of stars it contains. Accordingly, we write $\mathscr{A} = \oplus_{N=0}^{\infty} \mathscr{A}_N$, and we have $\partial \mathscr{A}_N \subset \mathscr{A}_{N-1}$.

Now, according to the expression of the kernel E_ν, the derivative d/dt of the value associated with a ν-star is given by

$$\frac{d}{dt}$$  $$= \alpha(t)\ \underbrace{\times\cdots\times}_{\nu},$$

this being true whatever may be the diagram in which this star is inserted. This implies that, for any regular diagram A (that is, not having any connected component reduced to a single cross), we have

$$\frac{d}{dt}\langle A\rangle = \alpha(t)\langle \partial A\rangle, \tag{1}$$

where $\langle A\rangle$ denotes the value of A.

Then, let us try to construct the retarded solution x of (E) under the form $x = \langle X\rangle$, where X is a combination of diagrams of the form

$$X = \times + \text{(regular terms)}. \tag{2}$$

In that expression, it will be necessary to admit a combination of an infinite number of terms. Thus the problem is posed in the (infinite) direct product

$$\bar{\mathscr{A}} = \prod_{N=0}^{\infty} \mathscr{A}_N,$$

which contains $\mathscr{A}$.[5] The corresponding value $\langle A\rangle$ of $A \in \bar{\mathscr{A}}$, then must be considered as a formal power series with respect to α. The equation (E) will be satisfied if we have

$$\partial X = P(X). \tag{3}$$

To solve this equation by a recursive process, let us introduce for any element A of $\bar{\mathscr{A}}$, the expansion

$$A = \sum_{N=0}^{\infty} A_N, \quad A_N \in \mathscr{A}_N,$$

so that (2) and (3) give

$$X_0 = \times, \tag{4}$$

$$\partial X_{N+1} = P(X)_N, \quad N \geqslant 0. \tag{5}$$

This last equation will furnish a solution for X_{N+1} in terms of the X_k, $0 \leqslant k \leqslant N$, which are the only ones occurring in the right-hand side, if one can show that $\partial : \mathscr{A}_{N+1} \to \mathscr{A}_N$ is surjective.

In fact, let us show that ∂ admits right inverses: Let M be any operator such as $[\partial, M] = 1$; if $D_N \in \mathscr{A}_N$ we can write

$$\frac{(-1)^{k-1}}{(k-1)!} M^{k-1}\partial^{k-1} D_N - \frac{(-1)^k}{k!} M^k \partial^k D_N = \frac{(-1)^{k-1}}{k!} \partial M^k \partial^{k-1} D_N. \tag{6}$$

Since $\partial^{N+1} D_N = 0$, by summing (6) over k, we obtain the identity[6]

$$D_N = \partial\left(\sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k!} M^k \partial^{k-1} D_N\right) = \partial\left(\sum_{k=1}^{N+1} \frac{(-1)^{k-1}}{k!} M^k \partial^{k-1} D_N\right).$$

By putting $D_N = P(X)_N$, this gives

$$X_{N+1} = \sum_{k=1}^{N+1} \frac{(-1)^{k-1}}{k!} M^k \partial^{k-1} P(X)_N, \tag{7}$$

which satisfies (5). It remains to exhibit an operator M such as $[\partial, M] = 1$. An immediate solution M_0 is given by $M_0(A) = \bullet A$, $\forall A \in \bar{\mathscr{A}}$. Since M_0 is simply the multiplication by the diagram $\bullet$, one easily verifies that the corresponding solution of (3) can be identified with the solution of the scalar equation

$$\frac{\partial}{\partial \alpha}\mathfrak{X} = P(\mathfrak{X}), \quad \mathfrak{X}(\alpha = 0) = \eta \tag{8}$$

by the correspondence rules

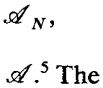
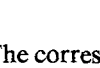
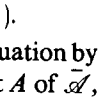
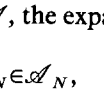
$$\bullet \to \alpha, \quad \times \to \eta,$$

where α and η are real variables, and $\mathfrak{X}$ is a function of these variables. However, such a solution does not satisfy (2). This condition will be satisfied if we choose M so that the transformed $M(A)$ of any diagram A is the diagram obtained by adding to A a point and joining it to each cross of A. With this definition, all the terms in the right-hand side of (7) indeed have a point joined to each cross and therefore are regular. This completes the proof of Theorem 1.

For example, the first few terms of the solution for

$$Px = (a/2)x^2 + (b/6)x^3$$

are given by

$$X = \times + \frac{a}{2}$$  $$+ \frac{b}{6}$$  $$+ \frac{a^2}{2}$$  $$- \frac{a^2}{4}$$  $$+ \frac{ab}{6}$$  $$- \frac{5ab}{24}$$  $$+ \frac{ab}{4}$$  $$+ \frac{b^2}{12}$$  $$- \frac{b^2}{24}$$  $$+ \cdots. \tag{9}$$

Passing to the retarded solution $x = \langle X\rangle$, we obtain the n-point functions:

$$G_2(t;\tau_1,\tau_2) = aE_2(t;\tau_1,\tau_2),$$

$$G_3(t;\tau_1,\tau_2,\tau_3) = bE_3(t;\tau_1,\tau_2,\tau_3) + 3a^2[\mathrm{sym}(E_2(t;\tau_1,\tau_2)E_3(t;\tau_1,\tau_2,\tau_3)) - \tfrac{1}{2}(E_3(t;\tau_1,\tau_2,\tau_3))^2],$$

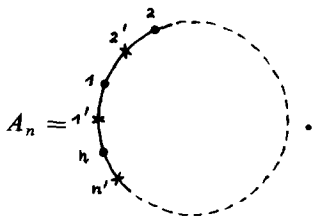
and so on.

One easily verifies that, as soon as the degree of P is greater than 1, diagrams with loops appear in each of the X_N's for $N > 1$; they come, for example, from the terms with $k \geqslant 2$ in (7) because of the form of the operator M. Theorem 2, that we now prove, allows a representation of $x(t)$ involving diagrams of a simpler structure, namely tree diagrams.

III. PROOF OF THEOREM 2

If $\langle A\rangle = \langle B\rangle$, $A, B \in \bar{\mathscr{A}}$, we say that the two elements A and B are equivalent, and write $A \simeq B$. Let us prove that any diagram A is equivalent to a linear combination of tree diagrams.

In a first step, let us consider the following diagram reduced to a loop:

$A_n =$ 

It will be necessary to distinguish the points (and the crosses) of A_n according to their labels, and consequently we denote as $\partial_k A_n$ the part of ∂A_n obtained by the derivation on the only point k. We then have

$$\partial A_n = \sum_{k=1}^{n} \partial_k A_n .$$

We shall show that A_n is equivalent to one combination of the diagrams obtained from A_n by suppressing some connecting lines of the type $(\alpha'\alpha)$, $1 \leqslant \alpha \leqslant n$. Such a term can be denoted by a symbol of the form $(B_{p_1} B_{p_2} \cdots B_{p_k})^m$, where B_p is the diagram

$B_p =$

p points,

lying along an arc of the loop A_n, and m is the rank in the sequence $B_{p_1} \cdots B_{p_k}$ of the point which coincides with the point of label 1.

The equivalence we want to show is $A_n \simeq C_n$ with

$$C_n = \sum_{k=1}^{n} \frac{(-1)^{k-1}}{k} \sum_{\substack{(p_1,\ldots,p_k) \\ p_j>1 \\ \sum_{j=1}^{k} p_j = n}} \sum_{m=1}^{n} (B_{p_1} \cdots B_{p_k})^m . \tag{10}$$

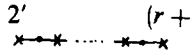
Clearly the right member of (10) is invariant under the cyclic permutations of $(1,2\cdots n)$. A further notation for the terms occurring in (10) is $B_{q_1}^{q} B_{q_2} \cdots B_{q_k}$, $1 \leqslant q \leqslant q_1$, where B_{q_1} is the section containing the point labeled 1, and q is the rank in the sequence $B_{q_1} \cdots B_{q_k}$ of this point. We have

$$(B_{p_1} \cdots B_{p_k})^m = B_{p_{l+1}}^{m-(p_1+\cdots+p_l)} \cdots B_{p_k} B_{p_1} \cdots B_{p_l},$$

with $p_1 + \cdots + p_l < m \leqslant p_1 + p_2 + \cdots + p_{l+1}$, so that the expression (10) becomes

$$C_n = \sum_{k=1}^{n} (-1)^{k-1} \sum_{\substack{(q_1,\ldots,q_k) \\ q_j>1 \\ \sum_{j=1}^{k} q_j = n}} \sum_{q=1}^{q_1} B_{q_1}^{q} \cdots B_{q_k} .$$

Denoting by D_r the diagram

$2' \quad (r+2)'$ 

lying along the loop, we have

$$\partial_1 C_n = \sum_{k=1}^{n} (-1)^{k-1} \sum_{\substack{(q_1,\ldots,q_k) \\ q_j>1 \\ \sum_{j=1}^{k} q_j = n}} \sum_{r=0}^{q_1-1} D_r B_{q_2} \cdots B_{q_k} B_{q_1-r-1}$$

$$= \sum_{r=0}^{n-1} D_r \sum_{l=0}^{n-1} \sum_{\substack{(p_1,\ldots,p_l) \\ p_i>1 \\ \sum_{i=1}^{l} p_i = n-r-1}} B_{p_1} \cdots$$

$$\times B_{p_l} [(-1)^l + (-1)^{l-1}(1-\delta_{l0})] .$$

The right member of the last equation is equal to $\partial_1 A_n$, so that $\partial_1 C_n = \partial_1 A_n$. Due to the cyclic invariance, this gives $\partial_k A_n = \partial_k C_n$, $1 \leqslant k \leqslant n$.

To continue to distinguish the points (and the crosses) in the value of the diagram, we have to affect, instead of α, different functions α_k, $1 \leqslant k \leqslant n$, to the different points, and not to integrate on the τ-variables attached to the crosses. The value so defined, denoted by $\langle\langle\ \rangle\rangle$, is then a kernel [containing the factor $\Pi_{i'} \theta(t - \tau_{i'})$]. Formula (1) for regular diagrams is generalized into

$$\frac{d}{dt} \langle\langle A \rangle\rangle = \sum_k \alpha_k(t) \langle\langle \partial_k A \rangle\rangle , \tag{11}$$

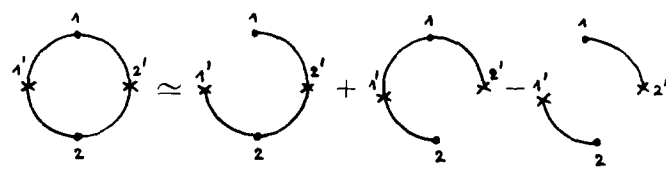
where k runs over the set of the points.

Since A_n and C_n are regular, formula (11) implies

$$\frac{d}{dt} \langle\langle An \rangle\rangle = \frac{d}{dt} \langle\langle C_n \rangle\rangle .$$

These functions being continuous and retarded, as can be easily verified, this yields the equality $\langle\langle A_n \rangle\rangle = \langle\langle C_n \rangle\rangle$ and finally $\langle A_n \rangle = \langle C_n \rangle$.

For example, for $n = 2$, we have the equivalence



(12)

and, between the corresponding kernels, the equality

$$\begin{aligned}
&(\overline{\alpha}_1(t) - \overline{\alpha}_1(\sup(\tau_1',\tau_2')))(\overline{\alpha}_2(t) - \overline{\alpha}_2(\sup(\tau_1',\tau_2'))) \\
&\quad = (\overline{\alpha}_1(t) - \overline{\alpha}_1(\tau_2'))(\overline{\alpha}_2(t) - \overline{\alpha}_2(\sup(\tau_1',\tau_2'))) \\
&\qquad + (\overline{\alpha}_1(t) - \overline{\alpha}_1(\sup(\tau_1',\tau_2')))(\overline{\alpha}_2(t) - \overline{\alpha}_2(\tau_1')) \\
&\qquad - (\overline{\alpha}_1(t) - \overline{\alpha}_1(\tau_2'))(\overline{\alpha}_2(t) - \overline{\alpha}_2(\tau_1')).
\end{aligned}$$

Thus, each loop of the type A_n can be replaced by a combination of diagrams deduced from A_n by suppressing one connection at least (open loops).

In a second step, let us consider the diagram A_n' obtained by adding to A_n an arbitrary number of crosses arbitrarily connected to some of the points k, $1 \leqslant k \leqslant n$, and let C_n' be the combination of diagrams then obtained by adding to each term in C_n the same crosses and connections. The equation $\partial_k A_n = \partial_k C_n$, $\forall k$, immediately implies $\partial_k A_n' = \partial_k C_n'$, and, therefore, $\langle\langle A_n' \rangle\rangle = \langle\langle C_n' \rangle\rangle$, then $\langle A_n' \rangle = \langle C_n' \rangle$.

The last step consists in considering an arbitrary diagram A in which a loop is distinguished. The subdiagram of A constituted by all the points of the loop and all the crosses connected to these points is of the type of A_n' considered above. This subdiagram is nothing but the set of the stars, the centers of which are the points of the loop. In the value $\langle\langle A \rangle\rangle$, this subdiagram contributes by the factor $\langle\langle A_n' \rangle\rangle$; since $\langle\langle A_n' \rangle\rangle = \langle\langle C_n' \rangle\rangle$, the same value $\langle\langle A \rangle\rangle$ is obtained by replacing in A the subdiagram A_n' by C_n'. In each of the

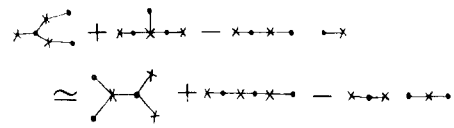
terms so obtained, the distinguished loop is open.

By iteration of this process, all the loops of any diagram A can be successively opened, that finally leads to a combination of tree diagrams. Q.E.D.

For example, the solution (9) for $P_{(x)} = (a/2)x^2 + (b/6)x^3$, is equivalent to X' with

$$X' = \times + \frac{a}{2} \; \text{---} + \frac{b}{6} \; \text{Y} + \frac{a^2}{4} \; \text{---} + \frac{ab}{24}\left[\text{---} \; \text{---} + 4 \; \text{---} \; \text{Y} \right] + \frac{b^2}{24} \; \text{Y} \; \text{---} \; \text{Y} + \cdots \qquad (13)$$

Remark: The equivalence $A_n \simeq C_n$ proved above privileges a rotation sense on the loop. Choosing the opposite sense furnishes, in general, a different equivalence $A_n \simeq \bar{C}_n$. When A_n is inserted into a larger diagram, the use of either of these equivalences may lead to different diagrams even after the removal of the labels of the points and of the crosses. In particular, this property can be used to obtain some equivalences between tree diagrams. For example, from (12), the two equivalences for the diagram  lead to the relation



Thus the representation of the solution $x(t)$ of (E) by a series of star diagrams is not unique, even when restricted to an expansion involving tree diagrams only.

Finally, let us notice that our results have not been obtained by a direct treatment of the equation (E); on the contrary we needed to introduce *a priori* the algebraic structure of abstract star diagrams, then to transpose in it the equation (E). This principle can be extended, and more general cases will be studied in a forthcoming paper.

[1] J. C. Houard, Lett. Nuovo Cimento **33**, 519 (1982).
[2] J. C. Houard and M. Irac-Astaud, J. Math. Phys. **24**, 1997 (1983).
[3] Here, we call a star that which was called a simple star in Ref. 2.
[4] The vanishing of α for $t < 0$ needs to be assumed when $P(0) \neq 0$ only; indeed, if $P(0) = 0$, the equation (E) is identically satisfied by $x(t) = 0$, $t < 0$, $\forall \alpha$.
[5] N. Bourbaki, *Eléments de Mathématique* (Hermann, Paris, 1955), Book II, Chap. II.
[6] When the operators M and ∂ are, respectively, replaced by the multiplication by x and the derivation d/dx, this identity reduces to a formula known for formal power series.

Formulas for the eigenvalues of the Laplacian on tensor harmonics on symmetric coset spaces

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(Received 13 March 1984; accepted for publication 8 June 1984)

On a symmetric coset space G/H the eigenvalues of the Laplacian and the Lichnerowicz operator acting on arbitrary tensor harmonics are given in terms of the eigenvalues of the quadratic Casimir operators of G and H. Explicit examples for S_n, CP_n, and real (complex) Grassmann manifolds are analyzed.

PACS numbers: 02.30.Tb

I. INTRODUCTION

In the Kaluza–Klein dimensional reduction of higher-dimensional gravity, gravity coupled to gauge fields, and supergravity,[1] the spectrum of the fields in the reduced model is given in terms of the eigenvalues of the differential operators acting on the internal compact space.[2–5] In most of the cases which have been considered the internal space is a coset manifold G/H, where G is a compact Lie group and H is its closed subgroup. The operators entering the mass formulas are usually the Laplacian $\Box$ and the Lichnerowicz operator Δ acting on tensors (spinors) of the internal space. The metric on G/H is G invariant. This implies that $\Box$ and Δ are also G invariant, so their eigenfunctions (eigentensors) fall into representations of G. It is convenient to expand all the fields into harmonics of G and G/H and then calculate the spectrum of $\Box$ and Δ. This program, proposed in Ref. 2 was later developed and applied both in gravity and supergravity models.[3–5]

In this paper we investigate the spectrum of the Laplacian and the Lichnerowicz operator acting on tensor (spinor) harmonics on G/H when G/H is a *symmetric* coset space (for a list of symmetric spaces see, e.g., Refs. 6 and 7). We show the following theorem.

Theorem: Let Y be a harmonic on G/H which transforms under an irreducible representation T (resp. D) of the group G (resp. H). Then the eigenvalues of $\Box$ and Δ are given by the following formulas:

$$\Box Y = [C_2^G(T) - C_2^H(D)]Y,$$

$$\Delta Y = C_2^G(T)Y,$$

where $C_2^G(T)$ [resp. $C_2^H(D)$] are the eigenvalues of the quadratic Casimir operators of T (resp. D).

This result is natural if one takes into account the G-invariance of $\Box$ and Δ. It was proved for some particular cases: for scalar harmonics,[7] for the Hodge–deRham operator acting on antisymmetric tensors on semisimple groups[8] and on S_n and CP_n (see Ref. 9), and for transverse, symmetric tensors on S_n (see Ref. 10), but we do not know about any other generalization. Thus we think it is useful to present here a short proof of it. It is given in Sec. II. Section III contains illustrative examples of the harmonics on spheres and Grassmann manifolds. In the Appendix we give algorithms for the calculation of Casimir operators on representations of unitary, orthogonal, and symplectic groups, which are simpler than those usually cited in the literature.

II. HARMONICS ON SYMMETRIC COSET SPACES

A harmonic on a coset space G/H in the irreducible representations T of G and D of H is defined as a function Y on the group G which satisfies the following properties[2,7,9]:

(i) $T(g)D(h)Y(g_0) = D(h)T(g)Y(g_0)$, $g_0, g \in G$, $h \in H$;

(ii) $Y(gg_0) = T(g)Y(g_0)$

(iii) $Y(g_0 h) = D(h^{-1})Y(g_0)$.

Consistency of (ii) and (iii) at the identity requires that the representation D appears in the branching of T under H. Usually one uses a particular representative of the harmonic which is a function on G/H. For this let us choose an embedding $L: G/H \to G$. To each point x of G/H, L assigns its representative $L(x)$ in G. (In general, L is defined only locally, and can be thought as a "coordinate system" on G/H.) Then the function Y^L, $Y^L(x) := Y(L(x))$ is the representation of Y in the gauge L. Using (ii) we see that the harmonic Y is completely determined by its value at the origin

$$Y(x) := Y^L(x) = T(L(x))Y(0), \quad 0 = eH. \tag{2.1}$$

The Lie algebra Γ of G can be decomposed into a simple sum $\Gamma = \Pi \oplus \Upsilon$, where Π is the Lie algebra of H and Υ is an Ad H-invariant subspace. Choosing a basis $\{t_M\} = \{t_i, t_\alpha\}$, $t_i \in \Pi$, $i = 1,\ldots,\dim H$, $t_\alpha \in \Upsilon$, $\alpha = 1,\ldots,n = \dim G/H$, the condition for G/H to be symmetric in terms of the structure constants $c_M{}^P{}_N$ ($[t_M, t_N] = c_M{}^P{}_N t_P$) is[6,7]

$$c_i{}^\alpha{}_j = c_i{}^j{}_\alpha = c_\alpha{}^\gamma{}_\beta = 0. \tag{2.2}$$

Let $\hat{\omega}^M = (\hat{\omega}^i, \hat{\omega}^\alpha)$ be the left invariant one-forms on G and $\omega^\alpha = L^* \hat{\omega}^\alpha$, $\omega^i = L^* \hat{\omega}^i$ their pullbacks onto G/H. On a symmetric space the $\omega^\alpha(x)$'s form a basis of the cotangent space at x and $\omega^\alpha{}_\beta = \omega^i c_i{}^\alpha{}_\beta$ is the Riemannian connection of the G-invariant metric g on G/H obtained from the invariant Killing metric on G by identifying Υ with the tangent space at $x = 0$ (see Refs. 6,7,11). In terms of the vielbein $e_\alpha(x)$, $\omega^\alpha(e_\beta) = \delta^\alpha{}_\beta$ this metric is given by

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$$g(e_\alpha(x), e_\beta(x)) = \eta_{\alpha\beta}, \tag{2.3}$$

where $\eta_{\alpha\beta}$ is the Killing form $\eta_{MN} = c\,\mathrm{Tr}(\mathrm{Ad}\,t_M\,\mathrm{Ad}\,t_N)$ restricted to Υ. For convenience one can choose this form so that it is proportional to δ_{MN}. This is always possible as G is compact.

The forms ω^i and ω^α can be found using the following expansion[2]:

$$L^{-1}\,dL = \omega^i t_i + \omega^\alpha t_\alpha. \tag{2.4}$$

Here H acts on the tangent space as a subgroup of SO(n). If we are interested in the expansion of tensor fields on G/H into harmonics the representation D must extend to a representation of SO(n).

The covariant derivative of Y along e_α is[6]

$$D_\alpha Y(x) = e_\alpha Y(x) + \omega_\alpha{}^i(x) D(t_i) Y(x). \tag{2.5}$$

From (2.4) in the representation T acting on e_α we get

$$e_\alpha T(L(x)) = T(L(x))[\omega_\alpha{}^i(x) T(t_i) + T(t_\alpha)]. \tag{2.6}$$

Thus (2.5) becomes simply

$$D_\alpha Y(x) = T(L(x)) T(t_\alpha) Y(0) = T(\mathrm{Ad}\,L(x) t_\alpha) Y(x). \tag{2.7}$$

Here we used that $T(t_i)Y(0) = -D(t_i)Y(0)$. From (2.6) for $T = \mathrm{Ad}$ we obtain

$$D_\alpha(\mathrm{Ad}\,L(x) t_\beta) = \mathrm{Ad}\,L(x)(c_\alpha{}^i{}_\beta t_i). \tag{2.8}$$

As $c_\alpha{}^i{}_\beta = -c_\beta{}^i{}_\alpha$

$$\eta^{\alpha\beta} D_\alpha T(\mathrm{Ad}\,L(x) t_\beta) = 0. \tag{2.9}$$

Thus the Laplacian on Y is

$$\Box Y(x) = \eta^{\alpha\beta} D_\alpha D_\beta Y(x) = \eta^{\alpha\beta} T(L(x)) T(t_\alpha) T(t_\beta) Y(0). \tag{2.10}$$

Now we observe that

$$\begin{aligned}\eta^{\alpha\beta} T(t_\alpha) T(t_\beta) Y(0) &= [\eta^{MN} T(t_M) T(t_N) - \eta^{ij} D(t_i) D(t_j)]\, Y(0) \\ &= [C_2^G(T) - C_2^H(D)]\, Y(0),\end{aligned} \tag{2.11}$$

which proves the first part of the Theorem.

The Lichnerowicz operator acting on a tensor harmonic $Y_{\alpha_1\cdots\alpha_k}$ (for simplicity of notation Y is a covariant tensor) is defined as follows[12]:

$$\Delta Y_{\alpha_1\cdots\alpha_k} = \Box Y_{\alpha_1\cdots\alpha_k} + \sum_{i=1}^{k} R^\alpha{}_{\alpha_i}{}^i{}_\alpha Y_{\alpha_1\cdots\alpha\cdots\alpha_k} + \sum_{\substack{i,j=1 \\ i\neq j}}^{k} R^\alpha{}_{\alpha_i}{}^\beta{}_{\alpha_j} Y_{\alpha_1\cdots\alpha\cdots\beta\cdots\alpha_k}. \tag{2.12}$$

Now let us recall that

$$D(t_i) Y_{\alpha_1\cdots\alpha_k} = -\sum_{j=1}^{k} c_i{}^\alpha{}_{\alpha_j} Y_{\alpha_1\cdots\alpha\cdots\alpha_k}{}^j. \tag{2.13}$$

The curvature and the Ricci tensor of the connection $\omega^\alpha{}_\beta$ are[11]

$$R^\alpha{}_{\beta\gamma\delta} = -c_\gamma{}^i{}_\delta c_i{}^\alpha{}_\beta, \quad R_{\beta\gamma} = R^\alpha{}_{\beta\gamma\alpha}. \tag{2.14}$$

It is easy to see that all the curvature terms in (2.12) sum up to

$$\eta_{ij} D(t_i) D(t_j) Y_{\alpha_1\cdots\alpha_k} = C_2^H(D) Y_{\alpha_1\cdots\alpha_k}. \tag{2.15}$$

Comparing it with (2.11) we obtain the second part of the Theorem.

When Y is a totally antisymmetric tensor the Lichnerowicz operator is equal to the Hodge–deRham operator. Thus our result agrees with Refs. 7 and 9.

In the next section we illustrate the Theorem with various examples. For this one needs to know how to construct harmonics on particular coset spaces. A general method can be found in Refs. 2 and 4. Here we outline it briefly.

Let $\Phi^A{}_B$ be matrices of some irreducible representation of the group G. Then

$$\Phi^A{}_B(gg_0) = \Phi^A{}_C(g)\Phi^C{}_B(g_0) = :T^A{}_C(g)\Phi^C{}_B(g_0), \tag{2.16}$$

$$\Phi^A{}_B(g_0 h^{-1}) = \Phi^A{}_C(g_0)\Phi^C{}_B(h^{-1}) = :D_B{}^C(h)\Phi^A{}_C(g_0). \tag{2.17}$$

In order to obtain a set of harmonics satisfying (i)–(iii) one must decompose the lower index into irreps of H. The basic formula for the covariant derivative of such harmonics follows from (2.17):

$$D_\alpha \Phi^A{}_B(x) = \Phi^A{}_C(x)\Phi^C{}_B(t_\alpha). \tag{2.18}$$

III. HARMONICS ON SPHERES, PROJECTIVE SPACES, AND GRASSMANN SPACES

In this section we will give an explicit construction of tensor harmonics on S_n, CP_n, and the real and complex Grassmann spaces

$$\begin{aligned} S_{pq} &= \frac{\mathrm{SO}(p+q)}{\mathrm{SO}(p)\otimes\mathrm{SO}(q)} \quad (p\geqslant q), \\ C_{pq} &= \frac{\mathrm{SU}(p+q)}{\mathrm{S(U}(p)\otimes\mathrm{U}(q))} \quad (p\geqslant q), \end{aligned} \tag{3.1}$$

with $CP_n = C_{n1}$ and $S_n = S_{n1}$. Harmonics on these spaces can be constructed as symmetrized tensor products of basic vector harmonics. We can calculate the eigenvalues of the Laplacian on these harmonics directly and thus demonstrate the general theorem.

In the following, SO $(p+q)$ and SU$(p+q)$ will be denoted generically as G, SO(p) and SU(p) as H_p, and SO(q) and SU(q) as H_q. Vector indices of G are denoted as $A,B,C,\ldots$, those of H_p as $a,b,c,\ldots$, and those of H_q as $\alpha,\beta,\gamma,\ldots$. Every vector V^A of G splits into two vectors V^a and V^α of H_p and H_q. The (anti-Hermitian) generators T_N of $\Gamma = H \oplus \Upsilon$ can be chosen in such a way that, in the vector representation of G,

$$\mathrm{Tr}(T_N T_M) = -2\,\delta_{NM}. \tag{3.2}$$

The generators of H and Υ are subsets of those of Γ.

We choose the following set of generators of Υ:

$$\begin{aligned} (T_{a\alpha})^A{}_B &= \delta_a^A \delta_{\alpha B} - \delta_\alpha^A \delta_{aB}, \quad \text{on } S_{pq}, C_{pq}, \\ (\overline{T}_{a\alpha})^A{}_B &= i(\delta_\alpha^A \delta_{aB} + \delta_a^A \delta_{\alpha B}), \quad \text{on } C_{pq}. \end{aligned} \tag{3.3}$$

These generators correspond to the components of the vectors of the tangent space group.

To define the Laplacian and Casimir operators we use the following invariant tensor:

$$\begin{aligned} \eta_{NM} &= \tfrac{1}{2}\mathrm{Tr}(T_N T_M), \quad S_{pq}, \\ \eta_{NM} &= \mathrm{Tr}(T_N T_M), \quad C_{pq}. \end{aligned} \tag{3.4}$$

This implies a choice of metric on these spaces [see (2.3)]. The Laplacian is in each case defined as

$$\Box = \sum_{N,M\in Y} \eta^{NM} D_N D_M = \begin{cases} \sum_{a\alpha} D_{a\alpha} D_{a\alpha}, & \text{on } S_{pq}, \\ \frac{1}{2} \sum_{a\alpha} (D_{a\alpha} D_{a\alpha} + \bar{D}_{a\alpha} \bar{D}_{a\alpha}), & \text{on } C_{pq}. \end{cases} \tag{3.5}$$

Using formula (2.18) we can calculate the effect of covariant derivatives on the matrices $\Phi^A{}_B$ of the vector representation of G. By splitting the index B into its H_p and H_q components we get the covariant derivatives on the harmonics $Y^A{}_b$ and $Y^A{}_\beta$:

$$\text{on } S_{pq}, C_{pq}, \quad D_{a\alpha} Y_\beta{}^A = \delta_{\alpha\beta} Y_a{}^A, \quad D_{a\alpha} Y^A_b = -\delta_{ab} Y^A_\alpha; \tag{3.6}$$

$$\text{on } C_{pq}, \quad \bar{D}_{a\alpha} Y^A_\beta = i\delta_{\alpha\beta} Y^A_a, \quad \bar{D}_{a\alpha} Y^A_b = i\delta_{ab} Y^A_\alpha.$$

Using (3.5) we find that on both spaces

$$\Box Y^A{}_b = -qY^A{}_b, \quad \Box Y^A{}_\beta = -pY^A{}_\beta. \tag{3.7}$$

Irreducible tensor harmonics can be obtained by multiplying N vector harmonics $Y^A{}_b$ with M vector harmonics $Y^A{}_\beta$, symmetrizing the three types of indices according to a set of Young diagrams, and subtracting traces if necessary. (The spaces S_{p2} and S_{p1} require a separate discussion, which will be given below.) The three Young diagrams specify irreducible representations R of G, r_p of H_p, and r_q of H_q. A harmonic exists only if the representation (r_p, r_q) of $H_p \otimes H_q$ is contained in R.

In the case of C_{pq} there is the additional requirement that the correct U(1) charge must be obtained. This can be achieved by considering all $U(p) \otimes U(q)$ representations (r'_p, r'_q) which contain (r_p, r_q) (r'_p differs from r_p by additional columns of length p). If $r'_p \otimes r'_q$ contains R, then R contains the representation (r_p, r_q) in its branching. (Rules for tensor products of Young diagrams are, for example, given in Refs. 13 and 14.) The correct U(1) charge can be obtained by adding the right number of columns to r_p and/or r_q. [There is of course a quantization condition for the U(1) charge which makes this possible.] A similar rule can be obtained for S_{pq}, but with the additional complication that a representation r_p or r_q can appear as a trace of a large representation. The precise formulation of this rule is not important for our purpose.

When $\Box$ acts on a properly symmetrized product of N basic harmonics Y^A_a and M harmonics Y^A_α there are contributions from $\Box$ acting on the factors in the product and "cross terms" with covariant derivatives acting on different factors. It is easy to show that in fact all cross terms between vector harmonics with the same type of lower index vanish. [For S_{pq} this is only true for those representations (r_p, r_q) that do not appear as trace terms. These trace terms require a separate discussion, but since our only purpose is to demonstrate the general result, which covers this case, this is not necessary. The case $q = 1$ also requires a separate discussion, which we will give below.]

The nonvanishing cross terms are

$$S_{pq}: \quad 2D_{a\alpha} Y^A_\beta D_{a\alpha} Y^B_b = -2Y^B_\beta Y^A_b,$$

$$C_{pq}: \quad D_{a\alpha} Y^A_\beta D_{a\alpha} Y^B_b + \bar{D}_{a\alpha} Y^A_\beta \bar{D}_{a\alpha} Y^B_b = -2Y^B_\beta Y^A_b. \tag{3.8}$$

This operation interchanges the upper indices of the harmonics. The sum of all such interchanges for the complete product can be expressed in terms of the operator Ω defined in the Appendix. Then we get, using (3.7):

$$\Box Y = (-(Nq + Mp) - 2\Omega_R + 2\Omega_p + 2\Omega_q)Y, \tag{3.9}$$

where $Y = Y(R, r_q, r_p)$ and Ω_R, Ω_p, and Ω_q act, respectively, on the G, H_p, and H_q indices of Y. Notice that the result is the same for S_{pq} and C_{pq}.

To compare with the Theorem we need the (properly normalized) Casimir operators on the representations R, r_p, and r_q. For the nonabelian groups these expressions are given in the Appendix. For S_{pq} one easily reproduces (3.9). For C_{pq} there is an extra contribution from the U(1) factor. In the vector representation of G, the U(1) charge, normalized according to (3.2) is

$$Q = \frac{i\sqrt{2}}{\sqrt{qp(q+p)}} \operatorname{diag}(q,\ldots,q,-p,\ldots,-p), \quad \text{with } \operatorname{Tr}(Q) = 0, \tag{3.10}$$

so that

$$QY(R, r_p, r_q) = \left[\frac{i\sqrt{2}}{\sqrt{pq(p+q)}}(Nq - Mp)\right] Y(R, r_p, r_q). \tag{3.11}$$

According to the Theorem we get then

$$\Box Y = \left[-(N+M)\left(p + q - \frac{(N+M)}{(p+q)}\right) + N\left(p - \frac{N}{p}\right) + M\left(q - \frac{M}{q}\right) + \frac{1}{qp(q+p)}(Nq - Mp)^2 - 2\Omega_R + 2\Omega_p + 2\Omega_q \right] Y. \tag{3.12}$$

This is indeed equal to (3.9).

Now we return to the special cases $q = 1$ and $q = 2$ for S_{pq}. The case $q = 2$ is special only because traceless tensors of SO(2) are not irreducible. All traceless symmetric tensor have two components, with "helicities" $\pm M$, for a tensor of rank M. Both components have the same Casimir eigenvalue, correctly given by (A7). Therefore the reducibility of these tensors is irrelevant, and (3.9) is valid.

As remarked before, if $q = 1$ there is an extra contribution due to cross terms among the scalar harmonics:

$$2D_a Y^A D_a Y^A = 2Y^A{}_a Y^A{}_a. \tag{3.13}$$

Here we have omitted the indices α, which can only take one value. This expression can be evaluated by using

$$\sum_{a=1}^{p} Y^A_a Y^B_a = \sum_{C=1}^{p+1} Y^A_C Y^B_C - Y^A Y^B = -Y^A Y^B \tag{3.14}$$

[the first term is equal to δ_{AB} and vanishes because the representations of $SO(p+1)$ are traceless]. Thus we get an extra contribution $M(M-1)$. Since the M scalar functions Y^A can only be in the completely symmetric representation, this cancels the term $2\Omega_q$ in (3.9). Therefore we get the following results for harmonics on a sphere S_p:

$$\Box Y(R,r) = [\, -(Mp + N) - 2\Omega_R + 2\Omega_r \,] Y(R,r), \tag{3.15}$$

where R and r are tensor representations of SO $(p+1)$ and SO (p) of rank $N+M$ and N.

These harmonics exist only if the Young diagram of R has in each column at least as many boxes as r, and at most one more. If R has precisely one extra box in each nontrivial column of r harmonic $Y(R,r)$ is transverse, i.e.,

$$D^{a_i} Y^{A_1 \cdots A_{N+M}}_{a_1 \cdots a_N} = 0 \quad (i = 1,\ldots,N). \tag{3.16}$$

This is a consequence of the fact that, according to (3.6), the divergence operation removes one box from r. For transverse harmonics the eigenvalue of $\Omega_R - \Omega_r$ can be calculated explicitly, and we obtain

$$\Box Y^T(r,M) = -(M^2 + M(p-1) - N) Y^T(r,M), \tag{3.17}$$

with r, N, and M as defined in (3.15). Remarkably, the eigenvalue depends only on the rank of the tensor corresponding to the representation r, not on the symmetry of its indices. Our result (3.17) agrees with the one obtained in Ref. 10 for transverse symmetric tensors.

After the completion of this manuscript we have found that our formula (2.11) has also been obtained by Strathdee.[15]

ACKNOWLEDGMENTS

We wish to thank P. van Nieuwenhuizen for comments.

This work was supported in part by National Science Foundation Grant No. PHY 81-09110 A-01.

APPENDIX: SIMPLE EXPRESSIONS FOR THE EIGENVALUES OF THE QUADRATIC CASIMIR OPERATOR FOR SO(N), SU (N), AND Sp (N)

In this appendix we present some simple expressions for the eigenvalues of the quadratic Casimir operator C_2 on representations of SO (N), SU (N), and Sp (N), defined with symmetrized tensors. We denote a tensor of rank r with indices symmetrized according to some Young diagram S as $T_{[\mu_1 \cdots \mu_r]S}$. We consider the following representations:

$$T_{[\mu_1 \cdots \mu_r]S}, \quad \text{SU } (N), \text{SO}(N), \text{ and Sp } (N), \tag{A1}$$

$$T_{\alpha[\mu_1 \cdots \mu_r]S}, \quad \text{SO } (N) \text{ (spinor representations)}.$$

Here μ_i is a vector index and α a spinor index. To obtain irreducible representations we must impose additional constraints:

$$\eta^{\mu_i \mu_j} T_{[\mu_1 \cdots \mu_r]S} = 0, \quad 1 \leqslant i \leqslant j \leqslant r, \tag{A2a}$$

$$\eta^{\mu_i \mu_j} T_{\alpha[\mu_1 \cdots \mu_r]S} = 0, \quad 1 \leqslant i \leqslant j \leqslant r, \tag{A2b}$$

$$\gamma^{\mu_i}_{\alpha\beta} T_{\beta[\mu_1 \cdots \mu_r]S} = 0, \quad 1 \leqslant i \leqslant j \leqslant r, \tag{A2c}$$

where $\eta^{\mu\nu}$ is the invariant tensor of SO(N) or Sp (N) and $\gamma^{\mu}_{\alpha\beta}$ are the Dirac matrices.

The Casimir operators on these representations can be expressed in terms of the following operator:

$$\Omega T_{[\mu_1 \cdots \mu_r]S} = \sum_{\text{pairs}} T_{[\mu_1 \cdots \mu_j \cdots \mu_i \cdots \mu_r]S}, \tag{A3}$$

i.e., Ω is the sum over the interchanges of all pairs of indices. Using the symmetry properties of Young diagrams (see, e.g., Ref. 13) one can show that the symmetrized tensors are eigenvectors of this operator, with eigenvalue

$$2\Omega_S = \sum_{i=1}^{n_r} f_i^2 - \sum_{i=1}^{n_c} g_i^2, \tag{A4}$$

where f_i and g_i are the length of the ith row and column of the Young diagram S, and n_r and n_r the number of rows and columns.

Consider first the group SO (N). We choose the following generators for the vector and spinor representation:

$$(M_{\rho\sigma})^{\mu}{}_{\nu} = \delta^{\mu}_{\rho}\delta_{\sigma\nu} - \delta^{\mu}_{\sigma}\delta_{\rho\nu}, \quad (M_{\rho\sigma})^{\alpha}{}_{\beta} = \tfrac{1}{4}[\gamma_{\rho},\gamma_{\sigma}]^{\alpha}{}_{\beta}. \tag{A5}$$

To get a normalization of the Casimir operator which is consistent with the results of Sec. III we use the invariant tensor (2.4), and obtain

$$C_2 = \tfrac{1}{2}\sum_{\rho,\sigma} M_{\rho\sigma} M_{\sigma\rho}. \tag{A6}$$

Acting on a symmetrized, traceless tensor of rank r this operator has the following effect:

$$C_2 T_{[\mu_1 \cdots \mu_r]S} = -(r(N-1) + 2\Omega) T_{[\mu_1 \cdots \mu_r]S}. \tag{A7}$$

To get the eigenvalues of C_2 on spinor representations we include extra terms coming from C_2 acting twice on the spinor index and once on a spinor and a vector index. These terms can be calculated easily with the help of (A2c). The result is

$$C_2 T_{\alpha[\mu_1 \cdots \mu_r]S} = -(rN + \tfrac{1}{8}N(N-1) + 2\Omega) T_{\alpha[\mu_1 \cdots \mu_r]S}. \tag{A8}$$

The calculation of the eigenvalues of C_2 for SU (N) and Sp (N) is completely analogous.[16] On the tensor defined in (A1) the eigenvalues are

$$\begin{aligned} &-(r(N - r/N) + 2\Omega), \quad \text{for SU } (N), \\ &-(r(N+1) + 2\Omega), \quad \text{for Sp } (N), \end{aligned} \tag{A9}$$

The Casimir operator in SU (N) has been normalized in agreement with Sec. III.

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A certain class of solutions of the nonlinear wave equation

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(Received 1 September 1981; accepted for publication 18 May 1984)

In this paper are investigated some differential geometry methods in the theory of the nonlinear wave equation $\nabla^2 u = \Phi(u,(\nabla u|\nabla u))$. A special class of solutions is discussed for which $(\nabla u|\nabla u)$ is constant on each level of the function u. It is proved that levels of such solutions form in the space of independent variable's hypersurfaces with all principal curvatures constant. The general form of such hypersurfaces is given. Then it is proved that via the method of characteristics it is possible to construct (in principle) all the solutions of the discussed class. They may be obtained by integration of an ODE of second order using a special class of the polynomial functions. Some new solutions are given for equations $\Box v = 4Av^3 + 3Bv^2 + 2cv + D$, $\Box v = \mu \exp v$, $\Box v = \sin v$, $\Box v = \cosh v$, *and* $\Box v = \sinh v$.

PACS numbers: 02.40. − k, 02.30.Jr

I. INTRODUCTION

Let $(\mathscr{E}, (\cdot|\cdot))$ be an n-dimensional ($n \geqslant 2$) pseudo-Riemannian manifold (i.e., the metric $(\cdot|\cdot)$ is nondegenerated but not necessarily positive definite). All functions, tensor fields, and manifolds are assumed smooth unless otherwise specified.

We shall consider partial differential equations (PDE) of the second order

$$\nabla^2 u = \Phi(u, (\nabla u|\nabla u)), \tag{1.1}$$

where $u:\mathscr{E}\to\mathbb{R}^1$ is a function of the class C^2, ∇u denotes the gradient of the function u, and ∇^2 is the Laplace–Beltrami operator[1,2] with respect to the metric $(\cdot|\cdot)$ (for instance in the Minkowski space $\nabla^2 = \Box$ is the d'Alembert operator, whereas for Euclidean space $\nabla^2 = \Delta$ is the usual Laplace operator). We are interested in the class of such solutions u of the equation (1.1) that $(\nabla u|\nabla u)$ is constant on every level of the function u, i.e., $(\nabla u|\nabla u) = \alpha(u)$, where α is an arbitrary function (of the class C^1) of one variable. Thus $\nabla^2 u = \Phi(u, \alpha(u)) =: \beta(u)$ is also the function constant on the levels of u, so

$$(\nabla u|\nabla u) = \alpha(u), \quad \nabla^2 u = \beta(u). \tag{1.2}$$

Let $u\to\vartheta(u) =: v$ be an arbitrary but invertible transformation of the dependent variable. Then

$$(\nabla v|\nabla v) = \vartheta'^2(u)\alpha(u) =: \tilde{\alpha}(v).$$

$$\nabla^2 v = \vartheta''(u)\alpha(u) + \vartheta'(u)\cdot\beta(u) =: \tilde{\beta}(v), \tag{1.3}$$

so the form of the system (1.2) remains unchanged. If α and β are treated as arbitrary functions then system (1.2) characterizes in fact the congruence of the levels of function u.

Note that if u satisfies the system (1.2) and ϑ is an integral of the second-order ordinary differential equation (ODE)

$$\alpha(u)\cdot\vartheta''(u) + \beta(u)\vartheta'(u) = \Phi(\vartheta(u), \alpha(u)\cdot\vartheta'^2(u)), \tag{1.4}$$

then, by (1.3), the superposition $v = \vartheta(u):\mathscr{E}\to\mathbb{R}$ satisfies

$$\nabla^2 v = \Phi(v, (\nabla v|\nabla v)).$$

Thus from each solution of the system (1.2) we can generate with help of the solution of Eq. (1.4) the two-parameter family of solutions of Eq. (1.1).

Next we shall consider the system (1.2). If $\alpha(u)\equiv 0$, then $(\nabla u|\nabla u) = 0$; the function u satisfying this equation will be called an isotropic one. This case will be investigated in Sec. V, whereas Secs. I–IV concern the nonisotropic case. Furthermore, if $\alpha(u)\not\equiv 0$ then [as is possible after the transformation $u\to v = \vartheta(u)$ with $\vartheta'(u) = |\alpha(u)|^{-1/2}$] we may assume that $\alpha(u) = \pm 1$.

II. GEOMETRICAL PROPERTIES OF THE LEVELS OF THE FUNCTION U

Further on we shall restrict ourself to the case of the flat space, i.e., when $\mathscr{E}$ is a vector space and $(\cdot|\cdot)$ is the symmetric nondegenerated bilinear form. The considerations below may be generalized to the case when $(\mathscr{E},(\cdot|\cdot))$ is a symmetric space (i.e., $\nabla_\lambda R^\mu{}_{\nu\rho\sigma} = 0$, see Ref. 2).

Consider the system of equations

$$(\nabla u|\nabla u) = \pm 1, \tag{2.1a}$$

$$\nabla^2 u = \beta(u), \tag{2.1b}$$

where β is an arbitrary function. In the language of the Grassmann algebra (2.1b) can be written in the form $\nabla(\nabla^2 u) \wedge \nabla u = 0$. Equation (2.1a) is of the Hamilton–Jacobi type. For the given values of the function u on a certain hypersurface $\Sigma \subset \mathscr{E}$ we can solve (2.1a) by the method of characteristics. In particular for the boundary condition

$$u|_\Sigma = 0, \tag{2.1c}$$

Σ will be one of the levels of the function u. The condition of transversality (that guarantees the local existence and uniqueness of the solution) for Eq. (2.1a) means that in every point of the hypersurface Σ there exists the nonisotropic [with respect to $(\cdot|\cdot)$] normal vector. The hypersurface Σ satisfying this condition will be called the nonisotropic one.

The method of characteristics[1] for the problem (2.1a) and (2.1c) gives the following result. For $x \in \Sigma$ let γ_x denote the straight line passing through x and normal to the hypersurface Σ parametrized in such a way that

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$$\gamma_x(0)=x \quad \text{and} \quad \left(\frac{d\gamma_x}{ds}\middle|\frac{d\gamma_x}{ds}\right)=\pm 1.$$

Let us assume also that the vectors $d\gamma_x(0)/ds$ have directions in accordance with the chosen orientation of the hypersurface Σ. In the more general case of symmetric spaces we must use geodetics instead of straight lines. If Σ is nonisotropic then the lines γ_x cover a certain neighborhood $\mathcal{O} \supset \Sigma$. That means that for $y \in \mathcal{O}$ there exists a uniquely determined point $x = x(y) \in \Sigma$ and the unique value of parameter s, such that $y = \gamma_x(s)$. In particular the function u defined by

$$\mathcal{O} \ni y \mapsto s := u(y), \quad \text{if } y = \gamma_x(s) \tag{2.2}$$

is a local solution of the problem (2.1a) and (2.1c). The choice of the second possible orientation on Σ gives us another (with the opposite sign) solution of the problem (2.1a), (2.1c)

Our aim is to determine the conditions which must be satisfied by the hypersurface Σ in order that the solution of the problem (2.1a) and (2.1c) would be also the solution of Eq. (2.1b). Therefore these conditions will characterize levels of the solution of the system (2.1a), (2.1b). The method of characteristics tells us how we can reconstruct the whole family of levels starting from the given one. That according to the remark from Sec. I gives us the general solution of the problem (1.2).

Theorem 1: A solution of the problem (2.1a), (2.1c) satisfies the equation (2.1b) iff a nonisotropic hypersurface Σ has all principal curvatures constant.

Proof: Let $u:\Sigma \subset \mathcal{O} \to \mathbb{R}^1$ be a solution of the problem (2.1a) and (2.1c). Denote $f := -\nabla^2 u$, $X := \nabla u$, and $D := -\nabla X$. Thus X is the tensor field of the type $\binom{1}{0}$ and D of the type $\binom{1}{1}$. The condition (2.1a) means that $(X|X) = \pm 1$. From the definition we conclude $(X|Y) = \nabla_Y u$ and $DY = -\nabla_Y X$ for an arbitrary vector field Y. First we show that[3] $\nabla_X X = 0$. Indeed, because of the symmetry of the Levi–Civita connection we have

$$\begin{aligned}&\nabla_X(X|Y)-\nabla_Y(X|X)\\ &\quad=(X|[X,Y])=(X|\nabla_X Y-\nabla_Y X).\end{aligned}$$

Thus, using $\nabla_Y(X|X) = 2(X|\nabla_Y X) = 0$ and the Leibniz rule we obtain that $(\nabla_X X|Y) = 0$ for arbitrary Y, hence $\nabla_X X = 0$. Using this result we can calculate

$$\begin{aligned}&(\nabla_X D)\cdot Y\\ &\quad=\nabla_X(DY)-D(\nabla_X Y)=-\nabla_X(\nabla_Y X)+\nabla_{\nabla_X Y}X\\ &\quad=-R(X,Y)\cdot X-\nabla_Y(\nabla_X X)-\nabla_{[X,Y]}X+\nabla_{\nabla_X Y}X\\ &\quad=-R(X,Y)\cdot X+\nabla_{\nabla_Y X}X\\ &\quad=-R(X,Y)\cdot X+D(DY),\end{aligned}$$

which means that $\nabla_X D = D^2 - R(X,\cdot)X$. We have assumed that the curvature vanishes so the last formula gives simply $\nabla_X D = D^2$. So by successive covariant differentiations of the equality $f = \operatorname{tr}(D)$ we obtain

$$(\nabla_X)^k f = k!\operatorname{tr}(D^{k+1}), \quad k \geqslant 0. \tag{2.3}$$

We shall see that there exists the polynomial of n-variables $\sigma_1,\ldots,\sigma_n$ (with constant coefficients) $W \in \mathbb{R}[\sigma_1,\ldots,\sigma_n]$ such that for

$$\sigma_k := \operatorname{tr}(D^k), \quad k \geqslant 0, \tag{2.4}$$

we have

$$\sigma_{n+1} = W(\sigma_1,\ldots,\sigma_n). \tag{2.5}$$

Let $\lambda_1,\ldots,\lambda_n$ denote eigenvalues of D (which are—in general—complex functions on $\mathcal{O}$); then

$$\sigma_k = \lambda_1^k + \cdots + \lambda_n^k. \tag{2.6}$$

On the other hand, coefficients τ_k of the characteristic polynomial

$$\lambda^n - \tau_1\lambda^{n-1} + \cdots + (-1)^n\tau_n = (\lambda-\lambda_1)\cdots(\lambda-\lambda_n)$$

of the tensor D are expressed as symmetric polynomials of variables $\lambda_1,\ldots,\lambda_k$:

$$\tau_k = \sum_{i_1<\cdots<i_k} \lambda_{i_1}\cdots\lambda_{i_k}. \tag{2.7}$$

Using (2.6) and (2.7) we obtain the following simple expression:

$$\tau_k = \frac{1}{k!}\cdot\begin{vmatrix}\sigma_1 & 1 & 0 & \cdots & 0\\ \sigma_2 & \sigma_1 & 2 & \cdots & 0\\ \sigma_{k-1} & \sigma_{k-2} & \sigma_{k-3} & \cdots & k-1\\ \sigma_k & \sigma_{k-1} & \sigma_{k-2} & \cdots & \sigma_1\end{vmatrix}, \quad k>0. \tag{2.8}$$

Since $\tau_{n+1} \equiv 0$, then for $k = n+1$ the expansion of this determinant with respect to the first column gives us an expression of the form (2.5).

It follows from (2.3)–(2.5) that the function $f = -\nabla^2 u$ satisfies the following PDE of nth order:

$$\frac{1}{n!}(\nabla_X)^n f = W\left(f, \nabla_X f, \ldots, \frac{1}{(n-1)!}(\nabla_X)^{n-1} f\right). \tag{2.9}$$

Note that the earlier investigated curves γ_x ($x \in \Sigma$) are integral trajectories of the fields X. So

$$\begin{aligned}\nabla_X f(\gamma_x(s)) &= \frac{d}{ds} f(\gamma_x(s)),\ldots,(\nabla_X)^n f(\gamma_x(s))\\ &= \frac{d^n}{ds^n} f(\gamma_x(s)).\end{aligned}$$

From Eq. (2.9) we obtain an ODE of the nth order for the function $s \to f(\gamma_x(s))$; thus f on some neighborhood of Σ is uniquely determined by the values $f, \nabla_X f, \ldots, (\nabla_X)^{n-1} f$ on the hypersurface Σ.

Since Eq. (2.9) has constant coefficients and [according to (2.2)] $u(\gamma_x(s)) = s$, one can express f as a function of u if and only if the functions $f|_\Sigma, \nabla_X f|_\Sigma, \ldots, (\nabla_X)^{n-1} f|_\Sigma$ are constant. This is exactly the case when f satisfies (2.1b). By virtue of (2.3), (2.4), and (2.8) the last condition is equivalent to the fact that $\tau_1,\ldots,\tau_n$ are constant on the hypersurface Σ.

To finish the proof we show that $\tau_n \equiv 0$ and that $\tau_1,\ldots,\tau_{n-1}$ are curvatures (i.e., principal invariants of the second fundamental tensor H[2,4,5]) of the hypersurface Σ. Let us consider the tensor $D|_\Sigma$. Because $D = -\nabla X$ and $n := X|_\Sigma$ is the field of unit normal vectors on Σ then $D \cdot v = H \cdot v$ for each vector v tangent to Σ. In turn $\nabla_X X = 0$ implies $D \cdot n = \nabla_X X|_\Sigma = 0$. Thus one of the eigenvalues of the tensor D vanishes (say $\lambda_n = 0$) while remaining ones (namely $\lambda_1,\ldots,\lambda_m$ where $m := n-1$) are eigenvalues of the second fundamental tensor of Σ (i.e., its principal curva-

tures). So $\tau_n = \lambda_1 \ldots \lambda_n = 0$ and $\tau_1, \ldots, \tau_m$ are curvatures of the hypersurface $\Sigma / (\tau_1/m) = (1/m)(\lambda_1 + \cdots + \lambda_m)$ and $\tau_m = \lambda_1 \cdots \lambda_m$ are known as mean and Gaussian curvatures. Q.E.D.

III. POLYNOMIAL SOLUTIONS OF THE SYSTEM $(\nabla u | \nabla u) = \alpha(u)$, $\nabla^2 u = \beta(u)$

We shall now find all solutions $u: \mathscr{E} \to \mathbb{R}^1$ of the system (1.2) of the special form

$$u(x) = \tfrac{1}{2}(Px|x) + (q|x) + u_0, \tag{3.1}$$

where $P = P^* \in \mathbb{L}(\mathscr{E}, \mathscr{E})$ is a symmetric [with respect to $(\cdot|\cdot)$] endomorphism, $q \in \mathscr{E}$ and $u_0 \in \mathbb{R}^1$. The importance of such solutions follows from the fact (proved in the next section) that each nonisotropic solution of (1.2) is of the form $v = \vartheta(u)$, where u is a polynomial solution (of degree $\leqslant 2$).

First we prove the following auxiliary.

Lemma1: If E_1, F are vector spaces and $P, Q \in \mathbb{L}(E_1, F)$ then the following conditions are equivalent.

(a) $Px \wedge Qx = 0$ for any $x \in E_1$.

(b) P and Q are proportional (i.e., $P = \lambda \cdot Q$ or $Q = \lambda \cdot P$) or $\operatorname{Im} P = \operatorname{Im} Q$ and $\operatorname{Im} P$ is a one-dimensional subspace of F.

Proof: Obviously (b) implies (a). Conversely, assume that (a) holds. We may assume that $P \neq 0$. Choose complementary subspaces E', F' for $K := \ker P$ and $I := \operatorname{Im} P$, respectively; thus $E_1 = E' \oplus K$, $F = I \oplus F'$, and P is of the form

$$P(e' \oplus k) = P'e' \oplus 0,$$

where $P' \in L(E', I)$ is an isomorphism. Putting $x = e' \oplus 0$ and $x = 0 \oplus k$ in (a) we see that Q must be of the form

$$Q(e' \oplus k) = (\lambda P'e' + Q_1 k) \oplus Q_2 k,$$

where $Q_1 \in \mathbb{L}(K, I)$, $Q_2 \in \mathbb{L}(K, F')$, and $\lambda \in \mathbb{R}^1$.

Now the condition (a) means that

$$Q_2 k = 0 \quad \text{and} \quad P'e' \wedge (\lambda P'e' + Q_1 k) = 0,$$

for any $e' \in E'$ and $k \in K$. Thus $Q_2 = 0$ and $i \wedge Q_1 k = 0$, for any $i \in I$ and $k \in K$. If $\dim I > 1$ (or if $Q_1 = 0$), the last condition implies $Q_1 = 0$ (that is $Q = \lambda P$). Otherwise $\dim I = 1$ and $\operatorname{Im} Q_1 = I$. That means that $\operatorname{Im} P = \operatorname{Im} Q = I$.

If I is a linear subspace of $\mathscr{E}$ we denote by $I^\perp$ its orthogonal [with respect to $(\cdot|\cdot)$] complement; I is called isotropic (respectively, nonsingular) iff $I \subset I^\perp$ (respectively, $I \cap I^\perp = \{0\}$, i.e., $I \oplus I = \mathscr{E}$). It follows from Witt's Theorem[6] that if $((+)^p, (-)^{n-p})$ is the signature of $(\cdot|\cdot)$ then the maximal dimension of isotropic subspaces is $\min(p, n-p)$.

Theorem 2: The polynomial u of degree $\leqslant 2$ is a solution of the system (1.2) iff u is (possibly after a transformation $u \to au + b$, $a \neq 0$) of one of the two following forms.

$$\text{(i)} \qquad u(x) = \frac{1}{2} \sum_{i=1}^{r} \epsilon_i (e_i|x)^2 + (q|x), \tag{3.2a}$$

where $(e_1, \ldots, e_r)$, $0 \leqslant r \leqslant \min(p, n-p)$, is a basis of an isotropic subspace $I \subset \mathscr{E}$, $q \in I^\perp$, and $\epsilon_i \in \{1, -1\}$, equivalently

$$(e_i|e_j) = 0, \ (e_i|q) = 0 \ \text{ for } i, j = 1, \ldots, r. \tag{3.2b}$$

$$\text{(ii)} \quad u(x) = \frac{1}{2} \sum_{i=1}^{r} \epsilon_i (e_i|x+q)^2, \tag{3.3a}$$

where $(e_1, \ldots, e_r)$, $1 \leqslant r \leqslant n$, is an orthornormal basis of a nonsingular subspace $I \subset \mathscr{E}$, $q \in I$, and $\epsilon_i = (e_i|e_i) \in \{1, -1\}$; i.e.,

$$(e_i|e_j) = \epsilon_i \delta_{ij},$$

$$\text{for } i, j = 1, \ldots, r, \quad q = \sum_{i=1}^{r} (e_i|q) e_i. \tag{3.3b}$$

Proof: If u is of the form (3.2a) or (3.3a) then simple calculation [using (3.2b) and (3.3b)] gives, respectively,

$$\nabla u(x) = \sum_{i=1}^{r} \epsilon_i (e_i|x) e_i + q, \quad (\nabla u | \nabla u)(x) = (q|q),$$

$$\nabla^2 u(x) = 0, \tag{3.2c}$$

and

$$\nabla u(x) = \sum_{i=1}^{r} \epsilon_i (e_i|x+q) e_i,$$

$$(\nabla u | \nabla u)(x) = \sum_{i=1}^{r} \epsilon_i (e_i|x+q)^2,$$

$$\nabla^2 u(x) = r. \tag{3.3c}$$

Thus if u is of the form (3.2a), it is a solution of the system (1.2) with

$$\alpha(u) = (q|q) \text{ and } \beta(u) = 0, \tag{3.2d}$$

while if u is of the form (3.3a), it is a solution of the system (1.2) with

$$\alpha(u) = 2u \quad \text{and} \quad \beta(u) = r. \tag{3.3d}$$

We shall now prove the other part of Theorem 2. Note that (3.1) implies $\nabla^2 u = \operatorname{tr} T$. Thus the second equation of (1.2) is automatically satisfied [with $\beta(u) = \text{const}$], while the first one gives us $P(Px+q) \wedge (Px+q) = 0$ [since $(\nabla u(x) = Px + q$ and $\nabla(\nabla u | \nabla u)(x) = 2P(Px+q)$].

Decomposing the left-hand side with respect to the powers of x we obtain the following equations which must hold for any x:

$$P^2 x \wedge Px = 0, \tag{3.4a}$$

$$P^2 x \wedge q + Tq \wedge Tx = 0, \tag{3.4b}$$

$$Tq \wedge q = 0. \tag{3.4c}$$

Since (3.4a) holds, we see with the help of Lemma 1 that the condition (b) is valid for P, $Q := P^2$ and $E_1 := : F := \mathscr{E}$. But if $I := \operatorname{Im} P$ is one dimensional then automatically $P^2 = \lambda P$ for some $\lambda \in \mathbb{R}^1$. Finally, (3.4a) is equivalent to $P^2 = \lambda P$, $\lambda \in \mathbb{R}^1$.

Now we consider two possible cases.

(i) If $\lambda = 0$ then $I = \operatorname{Im} P \subset \ker P = (\operatorname{Im} P^*)^\perp = I^\perp$ and, therefore I is an isotropic subspace. Equation (3.4c) means that q is an eigenvector of P with the eigenvalue λ. Thus $Pq = 0$, i.e., $q \in I^\perp$. Since (3.4b) also holds, it remains to describe the form of the operator P. Let us choose a basis $(e_1, \ldots, e_r)$ in I. Then $Px = \Sigma_{i=1}^r (P_i|x) e_i$, where the P_i are vectors in $\mathscr{E}$. But $\ker P = I^\perp$, which means that $P_i \in (I^\perp)^\perp = I$ and the P_i are linearly independent. Hence $P_i = \Sigma_{j=1}^r p_{ij} e_j$, where $\|p_{ij}\|$ is a nonsingular and symmetric matrix. The last statement is a consequence of the symmetry of P. A change of the basis (e_i) transforms the coefficients p_{ij} as coefficients of a bilinear form. Thus (e_i) may be chosen in such a way that $p_{ij} = \epsilon_i \delta_{ij}$, $\epsilon_i = \pm 1$. Then $Px = \Sigma_{i=1}^r \epsilon_i (e_i|x) e_i$ and consequently, (3.2a) and (3.2b) hold.

(ii) If $\lambda \neq 0$ (and $P \neq 0$) then we may multiply u by $1/\lambda$ and, consequently we may assume that $\lambda = 1$. Thus $P^2 = P$, i.e., P is an (orthogonal) projection. In particular, $\mathscr{E} = \operatorname{Im} P \oplus \ker P = I \oplus I^{\perp}$, i.e., I is a nonsingular ($\neq 0$) subspace. Formula (3.4b) means that $Px \wedge (\mathbf{1} - P)q = 0$ for any x. Thus $(\mathbf{1} - P)q \in I$ and, since $\operatorname{Im}(\mathbf{1} - P) = I^{\perp}$, one has $(\mathbf{1} - P)q = 0$, that is, $q \in I$. Hence (3.4c) holds. Moreover

$$\tfrac{1}{2}(P(x+q)|(x+q)) = \tfrac{1}{2}(Px|x) + (q|x) + \tfrac{1}{2}(q|q)$$

equals the right-hand side of (3.1) modulo and additive constant. If we choose an orthonormal basis $(e_1,\ldots,e_r)$ of I, this expression is equal to $\frac{1}{2}\sum_{i=1}^{r} \epsilon_i (e_i|x+q)^2$. This ends the proof.

Q.E.D.

Remark: If $\mathscr{E}$ is an $(m+1)$-dimensional vector space with coordinates $(x^0,\ldots,x^m)$ and

$$(x|y) := x^0 y^0 - \sum_{i=1}^{r} x^i y^i,$$

then Theorem 2 says that all polynomial solutions (of degree $\leqslant 2$) of (1.2) may be obtained from the list[7,8]

$$u(x) = x^0, \quad u(x) = (x^0 \pm x^1),$$

$$u(x) = x^1, \quad u(x) = \frac{1}{2}\sum_{i=1}^{r} x^{i2} \quad 1 \leqslant r \leqslant m, \tag{3.5}$$

$$u(x) = \frac{1}{2}(x^0 \pm x^1)^2 + x^2, \; u(x) = \frac{1}{2}(x^{02} - \sum_{i=1}^{r} x^{i2}),$$

$$0 \leqslant r \leqslant m,$$

$$u(x) = \tfrac{1}{2}(x^0 \pm x^1)^2$$

by applying an isometry (i.e., Poincaré's transformation) to $x - es$ and linear (i.e., of the form $u \to au + b$) transformations in the dependent variable u.

Example: Consider the system of PDE's

$$\nabla^2 v = 0, \tag{3.6a}$$

$$(\nabla v|\nabla v) = a(v), \tag{3.6b}$$

where $a(\cdot)$ is a given function. According to (1.4) and (3.2d), if we substitute $v = \vartheta(u)$, where u is of the form (3.2a) [with $(q|q) \neq 0$] into (3.5a) and (3.5b), we obtain the ODE $\vartheta''(u) = 0$. Thus

$$v = \vartheta(u) = C \cdot u + v_0, \tag{3.7}$$

and [since (1.3) holds] $a(v) = C^2(q|q) = \text{const}$.

Similarly, if u is as in (3.3a) then $2u \cdot \vartheta''(u) + r\vartheta'(u) = 0$. Therefore

$$v = \vartheta(u) = \begin{cases} C \cdot |u|^{1-r/2} + v_0, & r \neq 2 \quad (3.8a) \\ C \cdot \ln|u| + v_0, & r = 2, \quad (3.8b) \end{cases}$$

and thus, again using (1.3), we obtain

$$a(v) = \begin{cases} \beta \cdot |v - v_0|^{2(r-1)/(r-2)}, & r \neq 2 \quad (3.9a) \\ \gamma \exp(kv), & r = 2, \quad (3.9b) \end{cases}$$

where β, v_0, k are real constants; moreover

$$|\beta| = 2(1 - r/2)^2 \cdot C^{2/(2-r)},$$

$$|\gamma| = 2C^2 \exp(v_0/C), \quad k = -1/C.$$

Thus it may be observed that if the function $a(\cdot) \not\equiv 0$ is such as in (3.8), then there exists a solution of (3.6) of one of the above-mentioned forms. Moreover, this solution is unique up to an isometric transformation in $\mathscr{E}$.

In the simplest case, when $\dim \mathscr{E} = 2$, it is easy to prove that all the solutions may be obtained in this way. Indeed, if $(\cdot|\cdot)$ has the signature $(+,+)$ then (3.6a) means that v is a real part of a holomorphic function f on $\mathscr{E}$, where we identify $\mathscr{E}$ with the complex plane $\mathbb{C}$. It follows from the Cauchy–Riemann equations that $(\nabla v|\nabla v) = |f'|^2$. Therefore (3.6b) implies

$$0 = d|f'|^2 \wedge d((f+\bar{f})/2) = \tfrac{1}{2}(f'^2\bar{f}'' - \bar{f}'^2 f'')d\bar{z} \wedge dz.$$

If $f' \neq 0, f''/f'^2$ is a real meromorphic function, i.e., $f''/f'^2 = -(1/f')' =: -2/C \in \mathbb{R}^1$. Therefore $f(z) = C\log((z - z_0)^2/2) + f_0$ and, hence

$$v(x,y) = \operatorname{Re} f(x+iy) = C \cdot \ln\frac{(x-x_0)^2 + (y-y_0)^2}{2} + v_0$$

is of the form (3.8b), while u is of the form (3.3a) with $r = 2$. Now $a(v) = 2C^2 \exp(-(v - v_0)/C)$, i.e., $a(v)$ is as in (3.9b). Furthermore, if $f'' = 0$ then f and, consequently, v are linear. Thus $v = C \cdot u + v_0$, where u is of the form (3.2a) with $r = 0$ [or $v = C \cdot |u|^{1/2} + v_0$, where u is as in (3.5a), with $r = 1$] and $a(v) = \text{const}$.

The case of $\sin(\cdot|\cdot) = (+,-)$ may be treated in a similar way by substituting $v(x,y) = f_1(x+y) + f_2(x-y)$ instead of $v = \operatorname{Re} f$. Our claim that the system (3.5) has solutions only if $a(\cdot)$ is of the form (3.9) and that in this case all its nonisotropic solutions may be obtained in the above described way [formulas (3.7) and (3.8)] remains true for $\mathscr{E}$ of any dimensions. That will follow from Corollary 1 which we introduce in the next section.

IV. HYPERSURFACE WITH CONSTANT PRINCIPAL CURVATURES

The aim of this section is to prove the following theorem.

Theorem 3: Let $(\mathscr{E}, (\cdot|\cdot))$ be an n-dimensional vector space with the nondegenerate scalar product $(\cdot|\cdot)$ and let $\Sigma \subset \mathscr{E}$ be such an $m = (n-1)$-dimensional nonisotropic hypersurface that all its principal curvatures $\lambda_1,\ldots,\lambda_m$ are constant. Then Σ may be described by an equation of one of the following forms:

(i) $u(x) := \frac{1}{2}(Px|x) + (q|x) = \text{const}$,

where $P \in \mathbb{L}(\mathscr{E}, \mathscr{E})$ is symmetric, $P^2 = 0$, and $q \in \ker P$ with $(q|q) = \pm 1$;

(ii) $u(x) := \frac{1}{2}(P(x - x_0)|(x - x_0)) = \text{const}$,

where $0 \neq P \in \mathbb{L}(\mathscr{E}, \mathscr{E})$ is symmetric, $P^2 = P$ (i.e., P is an orthogonal projection), and $x_0 \in \mathscr{E}$.

It follows from consideration of Secs. II and III (and may be easily checked by straightforward calculations) that hypersurfaces given by equations of form (i) or (ii) have constant curvatures; thus the converse theorem is also true.

Corollary 1: Each nonisotropic solution v of the system PDE

$$(\nabla v|\nabla v) = \alpha(v), \quad \nabla^2 v = \beta(v)$$

has (at least locally) the form $v = \vartheta(u)$, where u is such as in Theorem 2.

Proof: It follows from Sec. II that the level $\Sigma := \{x/v(x) = v_0\}$ of such solution has all its principal curvatures constant. So Σ is such as in Theorem 3, say (for instance) $\Sigma = \{x/u(x) = x_0\}$ is of the form (i). Let $\vartheta(\cdot)$ be the solution

of the problem $\vartheta'^2(u)=\alpha(\vartheta(u))$, $\vartheta(u_0)=v_0$. Then $(\nabla\vartheta(u)|\nabla\vartheta(u)=\alpha(\vartheta(u))$ and $\vartheta(u)|_\Sigma=\vartheta(u_0)=v_0=v|_\Sigma$. So $\vartheta(u)=u$ (in some neighborhood of Σ) by virtue of the uniqueness of the solution of the boundary problem for the equation $(\nabla v|\nabla v)=\alpha(v)$. The case when Σ is of the form (ii) may be treated in a similar way.

For simplicity we limit our considerations to the case when $(\cdot|\cdot)$ is positive-definite. The case of an indefinite metric is difficult because of the existence of symmetric tensors that cannot be diagonalized (the Classification Theorem about such tensors may be found in Ref. 9). For instance, hypersurfaces Σ of the form (i) with $P\neq 0$ have all principal curvatures vanishing. On the other hand, the second fundamental tensor H of such a Σ is in any point $x\in\Sigma$ the restriction of P to the subspace $T_x\Sigma$ and thus it is not a vanishing nilpotent operator. It is a rather surprising fact that if in addition rank $P=1$, then such a quadratic Σ may be isomorphically mapped onto the hyperplane $\langle q\rangle^\perp$; such an isomorphism is given by $\Sigma\ni x\mapsto x-\epsilon\cdot(q|x)(q+\frac{1}{2}Px)\in\langle q\rangle^\perp$ (where $\epsilon:=(q|q)=\pm 1$), which may be easily checked by virtue of the identity $(Px|x)(Py|y)=(Px|y)^2$.

Let S be an immersed submanifold of dimension l in $\mathscr{E}$ and let $\epsilon>0$. Denote for $s\in S$,

$$\Sigma_s:=\{x\in\mathscr{E}/x-s\in(T_sS)^\perp,\ |x-s|=\epsilon\},\tag{4.1}$$

the $(m-l)$-dimensional sphere with center s laying in the hyperplane perpendicular to T_sS. Let us define

$$\Sigma:=\bigcup_{s\in S}\Sigma_s,\quad \pi:\Sigma\to S,\quad \pi|_{\Sigma_s}:=s.\tag{4.2}$$

If ϵ and S are "sufficiently small" (namely, so that the below described endomorphism I_x of $T_{\pi(x)}S$ is invertible for any $x\in\Sigma_s$, $s\in S$) then Σ is an immersed hypersurface, π is a submersion, and the triple (π,Σ,S) is a fibered bundle with an $(m-l)$-sphere as a typical fiber. So constructed, Σ will be called the ϵ-tube around the submanifold S.

Lemma 2: Let $\Sigma\subset\mathscr{E}$ be a hypersurface having constant principal curvature $\lambda\neq 0$ with multiplicity $k\geqslant 1$ [i.e., $V:=\ker(H-\lambda\mathbb{1})$ is an k-dimensional distribution on Σ]. Define a mapping

$$\pi:\Sigma\to\mathscr{E},\quad \pi(x):=x+(1/\lambda)n(x),\tag{4.3}$$

where n is the normal unit vector on Σ, and let $S:=\pi(\Sigma)\subset\mathscr{E}$. Then S is an immersed submanifold of dimension $l:=m-k$ and Σ is an open subset of the ϵ-tube around S (with $\epsilon:=1/|\lambda|$).

Proof: It follows from the definition of the second fundamental tensor[2,5] H that the differential of π is $d\pi(x)\cdot\delta x=\delta x-(1/\lambda)H_x\cdot\delta_x$, i.e., $d\pi(x)=\mathbb{1}-(1/\lambda)H_x$. Thus $\ker d\pi(x)=V_x$ is the k-dimensional subspace of eigenvectors of H_x corresponding to eigenvalue λ. Therefore we see from the Rank theorem[1,2,5] that S is an immersed submanifold of dimension $l=m-k$ and the fibers of π are k-dimensional submanifolds on Σ.

Using the symmetry of S for $s=\pi(x)$ we obtain

$$\begin{aligned}T_sS&=\mathrm{Im}(\mathbb{1}-(1/\lambda)H_x)\\&=T_x\Sigma\ominus\ker(\mathbb{1}-(1/\lambda)H_x)=T_x\Sigma\ominus V_x;\end{aligned}$$

thus $n(x)\in(T_sS)^\perp$ and, since $x-s=-(1/\lambda)n(x)$,

$$x-s\in(T_sS)^\perp,\quad |x-s|=\epsilon,\quad \text{for } x\in\pi^{-1}(s),\tag{4.4}$$

that is, $\pi^{-1}(s)\subset\Sigma_s$ in accordance with (4.1). It proves that Σ is contained in the ϵ-tube around S and (because of equality of dimensions) it is its open subset.

Q.E.D.

Lemma 3: Let Σ be an ϵ-tube around an l-dimensional submanifold $S\subset\mathscr{E}$. Thus Σ has all principal curvatures constant iff S is flat (i.e., it is an open subset of an l-dimensional plane in $\mathscr{E}$).

Proof: Denote by $\mathscr{H}$ the second fundamental tensor of S. It means that for $s\in S$, $\mathscr{H}_s$ is a bilinear map

$$\mathscr{H}_s:(T_sS)^\perp\times T_sS\to T_sS,\quad (r,\delta s)\to\mathscr{H}_s(r,\delta s),$$

which may be defined by

$$\mathscr{H}_{s(t)}(r(t),\dot s(t)):=-\dot r(t)^T,\tag{4.5}$$

where $s(t)$ is a curve on S, $r(t)\in(T_{s(t)},S)^\perp$, and the symbol $(\cdot)^T$ denotes the tangent to S component of the vector.[10]

Now we express the second fundamental tensor H of the hypersurface Σ by the tensor $\mathscr{H}$. Because Σ has (induced from $\mathscr{E}$) Riemannian structure, then for $x\in\Sigma_s\subset\Sigma$ we have

$$T_x\Sigma=\langle n(x)\rangle^\perp=T'_x\Sigma\oplus T^-_x\Sigma,\tag{4.6}$$

where $n(x):=-\lambda(x-\pi(x))$ is the normal unit vector with $\lambda=\pm 1/\epsilon$ (the $+$ sign corresponds to internal and the $-$ sign to external orientation of Σ). The subspaces

$$T'_x\Sigma:=T_x\Sigma_s=\langle T_sS,x-s\rangle^\perp,\quad T^-_x\Sigma:=T_sS\tag{4.7}$$

are the vertical and horizontal components of $T_x\Sigma$.

Let us denote by $I_x:T_sS\to T^-_x\Sigma=T_sS$ the operator of horizontal lifting,[2,5] i.e.,

$$I_x:=(d\pi(x)|_{T^-_x\Sigma})^{-1}.$$

Now we determine the explicit form of I_x.

It is well known that any curve $s(t)$ in S may be lifted to a horizontal curve in Σ, i.e., such that $\dot x(t)\in T^-_{x(t)}\Sigma$. Putting $x(t)=s(t)+r(t)$ we have $r(t)\in(T_{s(t)}S)^\perp$, whereas [since $\dot s(t)\in T_{s(t)}S=T^-_{x(t)}\Sigma$] the horizontality condition means that $\dot r(t)\in T_{s(t)}S$. Thus $\dot r(t)=\dot r(t)^T$ and (4.5) gives

$$\dot x(t)=\dot s(t)+\dot r(t)=\dot s(t)-\mathscr{H}_{s(t)}(x(t)-s(t),\dot s(t)).\tag{4.8}$$

It is the ODE on the horizontal lifting or curves in S. Since $s(t)$ was an arbitrary curve, it follows from (4.8) that the horizontal lifting of vector δ_s is the vector

$$\delta_x=I_x\cdot\delta_s=\delta_s-\mathscr{H}_s(x-s,\delta_s).$$

Thus

$$I_x=\mathbb{1}-\mathscr{H}_s(x-s,\cdot)=:\mathbb{1}-J_x.\tag{4.9}$$

Now, from the definition of H, we have $H_{x(t)}\dot x(t)=-\dot n(t)$, where $n(t)=-\lambda(x(t)-s(t))$. Thus, consideration of the vertical curves [i.e., such that $s(t)=\mathrm{const}$] and horizontal ones [i.e., such that (4.8) holds] by virtue of (4.8) gives

$$H_x\cdot\delta_x=\begin{cases}\lambda\cdot\delta_x, & \text{if } \delta_x\in T'_x\Sigma \text{ is vertical,}\\ \lambda\cdot J_x\delta_s, & \text{if } \delta_x=I_x\delta_s \text{ is horizontal.}\end{cases}$$

So, since (4.6) and (4.9), H_x has the eigenvalue λ with multiplicity $k=m-l$ and its remaining eigenvalues are $-\lambda j_\alpha(x)/(1-j_\alpha(x))$, where $j_\alpha(x)$, $(\alpha=1,\ldots,l)$ are eigenvalues of the tensor $J_x=\mathscr{H}_s(x-s,\cdot)$.

Thus, because $\mathscr{H}_s$ linearly depends on $x-s\in(T_sS)^\perp$, the eigenvalues of H are constant iff $\mathscr{H}\equiv 0$. The last condi-

tion, in turn, implies that S is flat (since the tangent space $T_s S$ is constant for $s \in \mathscr{E}$).

Q.E.D.

Proof of Theorem 3: If all principal curvatures of Σ vanish, then Σ is flat, i.e., it satisfies an equation of the form $(q|(x - x_0)) = 0$. This is the case (i) of our theorem. Otherwise, there exists nonzero curvature λ and it follows from Lemma 2 that Σ is an open subset of the ϵ-tube ($\epsilon = 1/\lambda$) around the submanifold $S = \pi(\Sigma)$. Lemma 3 in turn says that S must be flat, i.e., it satisfies an equation of the form $P(x - x_0) = 0$, where P is an orthogonal projection. Thus the ϵ-tube around S is given by $(P(x - x_0)|(x - x_0)) = \epsilon^2$, which gives us the case (ii) of the Theorem.

Q.E.D.

V. ISOTROPIC SOLUTIONS OF NONLINEAR WAVE EQUATION

In this section we shall study isotropic [i.e., those that satisfy the Hamilton–Jacobi equation for massless particles $(\nabla u|\nabla u) = 0$] solutions of the nonlinear wave equation (1.1). It follows from the theorem below that (1.1) possesses isotropic solutions only for the very special case when $\Phi(u, 0) \equiv 0$.

Theorem 4: Let $\mathscr{E}$ be a $n = (m + 1)$-dimensional Minkowski space with the metric $(\cdot|\cdot)$ of the signature $(1, m)$. Then for the function u (of the class C^3) defined in some neighborhood of $0 \in \mathscr{E}$ the following conditions are equivalent.

(a) u satisfies the equations

$$(\nabla u|\nabla u) = 0, \quad \nabla^2 u = 0. \tag{5.1}$$

(b) u is a solution of the system

$$(\nabla u|\nabla u) = 0, \quad \nabla^2 u = \beta(u) \tag{5.2}$$

for a certain function β.

(c) u satisfies the equations

$$(\nabla u|\nabla u) = 0, \quad (\nabla(\nabla^2 u)|\nabla u) = 0. \tag{5.3}$$

(d) $x \to u(x)$ may be defined in the implicit form by the equation

$$F((w(u)|x)) = u, \tag{5.4}$$

where $F(\cdot)$ is a real function of one variable and $u \to w(u) \in \mathscr{E}$ is a one-parameter family of nonzero isotropic vectors.

Proof: Obviously (a) $\Rightarrow$ (b) and, since $(\nabla\beta(u)|\nabla u) = \beta'(u)(\nabla u|\nabla u)$, (b) $\Rightarrow$ (c). Further, differentiating (5.4) we have

$$F'((w|x)) \cdot ((w'|x)\nabla u + w) = \nabla u,$$

$$F''((w|x)) \cdot ((w'|x)\nabla u + w|(w'|x)\nabla u + w) + F'((w|x))((w'|x)(\nabla u|\nabla u) + 2(w'|\nabla u) + (w'|x)\nabla^2 u) = \nabla^2 u.$$

Thus

$$\nabla u = \frac{F'((w|x))w}{1 - F'((w|x)) \cdot (w'|x)}$$

is isotropic and, because $(w(u)|w(u)) = 0$ implies $(w'(u)|w(u)) = 0$, $\nabla^2 u = 0$. Therefore (d) $\Rightarrow$ (a) and it remains to prove that (c) $\Rightarrow$ (d).

Let $(x^0, x^1, \ldots, x^m)$ denote Cartesian coordinates in $\mathscr{E}$ such that $(x|y) = x^\mu y_\mu = x_0 y_0 - x_i y_i$. Here and in the sequel we shall use the Einstein convention, that is, repeated indices denote summation over their range ($\lambda, \mu, \nu, \ldots \in \{0, \ldots, m\}$ and $i, j, k, \ldots \in \{1, \ldots, m\}$).

We use also standard notation

$$u_\mu := \frac{\partial u}{\partial x^\mu}, \quad u_{\mu\nu} := \frac{\partial u}{\partial x^\mu \partial x^\nu}, \quad u^0 := u_0,$$

$$u^i := -u_i, \quad u^i{}_\mu := -u_{i\mu}, \text{ etc.}$$

Let us assume that u satisfies condition (c). Differentiating the isotropy condition $u^\lambda u_\lambda = 0$, we have

$$u^\lambda u_{\lambda\mu} = 0, \quad u^\lambda u_{\lambda\mu\nu} + u^\lambda{}_\mu u_{\lambda\nu} = 0. \tag{5.5}$$

Thus the second equation of the system (5.3), that is, $u^\lambda u_\lambda{}^\mu{}_\mu = 0$, may be rewritten in the form

$$u^\lambda{}_\mu u^\mu{}_\lambda = 0. \tag{5.6}$$

If $u = \text{const}$ then (5.4) holds with $F = \text{const}$. Therefore we may assume that $\nabla u \neq 0$, i.e., $u_0 = \pm\sqrt{u_i u_i} \neq 0$. Then from (5.5) we obtain the following formulas:

$$u_{0i} = (1/u_0)u_{ij}u_j, \quad u_{00} = (1/(u_0)^2 u_{ij}u_i u_j, \tag{5.7}$$

so (5.6) may be expressed as

$$0 = (u_{00})^2 - 2u_{0i}u_{0i} + u_{ij}u_{ij} = (u_{ij}n_i n_j)^2 - 2u_{ik}u_{kj}n_i n_j + u_{ij}u_{ij}, \tag{5.8}$$

where $n_i := u_i/u_0$. Now we shall show that (5.8) describes the fact that all the levels of the function u are hyperplanes in $\mathscr{E}$. For this purpose observe that for $\rho \in \mathbb{R}^1$ and

$$\gamma_i := u_{ij}n_j - \rho n_i, \tag{5.9}$$

we have the following identity:

$$\sum_{i,j=1}^{m} (u_{ij} - \gamma_i n_j - \gamma_j n_i)^2 = 4\rho^2 - 4(u_{ij}n_i n_j)\rho + (2(u_{ij}n_i n_j)^2 - 2u_{ik}u_{kj}n_i n_j + u_{ij}u_{ij}).$$

By (5.8) it reduces to

$$\sum_{i,j=1}^{m} (u_{ij} - \gamma_i n_j - \gamma_j n_i)^2 = (2\rho - u_{ij}n_i n_j)^2,$$

which means that

$$u_{ij} = \gamma_i n_j + \gamma_j n_i \tag{5.10}$$

for γ_i given by (5.9) with $\rho = \frac{1}{2}u_{ij}n_i n_j$. Thus, using (5.7) we obtain

$$u_{\mu\nu} = \beta_\mu u_\nu + \beta_\nu u_\mu, \tag{5.11}$$

where $\beta_0 := (1/2u_0)u_{ij}n_i n_j$ and $\beta_i := \gamma_i/u_0$. Now observe that if X is a vector field on $\mathscr{E}$ tangent to the levels of u (i.e., such that $u_\mu X^\mu = 0$) then (5.11) gives

$$\nabla_X u_\mu = u_{\mu\nu}X^\nu = (\beta_\nu X^\nu)u_\mu.$$

Hence the gradient ∇u has constant direction on each level of u (at least in the local sense). Thus $\nabla u = \varphi \cdot w(u)$ for a certain function $\varphi \neq 0$ and some one-parameter family of isotropic vectors $w(u) \in \mathscr{E}$. Therefore

$$\nabla(w(u)|x) = [(w'(u)|x) + 1/\varphi]\nabla u,$$

and thus the function u may be expressed as a function on $(w(u)|x)$, i.e., $u = F((w(u)|x))$ for a certain function $F(\cdot)$

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Remark 1: The rather surprising fact that (b) implies (a) simply means that $\beta \equiv 0$ is the compatibility condition for the system (5.2).

Remark 2: In the more general case of an arbitrary signature of $(\cdot \mid \cdot)$ let us assume that, for $u \in \mathbb{R}^1$, $(w^1(u),...,w^r(u))$ form the basis of an isotropic subspace $I(u) \subset \mathscr{E}$ and let $F(\cdot,...,\cdot)$ be a real function of r variables. Then it is easy to check that the function $x \to u(x)$, defined in implicit form by the equation

$$F((w^1(u)|x),...,(w^r(u)|x)) = u, \tag{5.12}$$

satisfies the system (5.1).

Our conjecture is that in such a way may be obtained a certain class of solutions of the system (5.1).

Remark 3: The characteristic peculiarity of functions u which may be described in the form (5.12) is that each their level $u(x) = u_0$ is the cylinder $F((w_0^1|x),...,(w_0^r|x)) = u_0$ [where $w_0^i = w^i(u_0)$], profiled by the level of F and with $\langle w_0^1,...,w_0^r \rangle^\perp$ as the generating subspace.

For the simplest case $r = 1$, (5.12) reduces to (5.4) and the cylinders become the hyperplanes.

In the theory of quasilinear PDE's solutions of the form (5.4) are known as Riemann waves whereas (5.14) defines the so-called nonplanar simple waves, cf. Refs. 11–13.

VI. EXAMPLES OF APPLICATION TO THE EQUATIONS OF MATHEMATICAL PHYSICS

Let us consider a particular form of Eq. (1.1), namely

$$\nabla^2 v = f(v). \tag{6.1}$$

Such equations can be found, for example, in the description of Josephson phenomenon in the Euclidean field theory, in the theory of elementary particles, in nonlinear electrodynamics, in magnetohydrodynamics, and in gasdynamics.

Substituting $v = \vartheta(u)$, where u is of the form (3.2), or (3.3a) leads to the following ODE:

$$\frac{d^2\vartheta}{du^2} = f(\vartheta), \tag{6.2a}$$

or

$$2u\frac{d^2\vartheta}{du^2} + \frac{d\vartheta}{du} = f(\vartheta), \tag{6.2b}$$

respectively [the coefficient $(q|q) \neq 0$ may be omitted in Eq. (6.2a) by including it in f]. If we exchange variable $s = \sqrt{2u}$ for $u > 0$ or $s = \sqrt{-2u}$ for $u < 0$ we can reduce Eq. (6.2b) to the Emden-type equations[14,15]

$$\frac{d^2\vartheta}{ds^2} + \frac{r-1}{s}\frac{d\vartheta}{ds} = \epsilon f(\vartheta), \quad \epsilon = \pm 1. \tag{6.3}$$

Note that if $r = 1$, then the above substitution transforms (6.3) to the form (6.2a). The ODE's (6.3) with $r \geqslant 2$ were investigated in papers[16,17] for some class of functions f. In particular when $r = 3$, in the literature[17,18] one can find existence theorems for solutions of (6.3) with properties $d\vartheta(0)/ds = 0$ and $\lim_{s\to\infty} \vartheta(s) = 0$ for their right-hand sides of the polynomial exponential and trigonometrical type

$$f(\vartheta) = \vartheta^n, \quad f(\vartheta) = \mu\vartheta + \lambda\vartheta^3, \quad f(\vartheta) = \exp\vartheta,$$
$$f(\vartheta) = \pm\sin\vartheta, \quad f(\vartheta) = \pm\cos\vartheta,$$
$$f(\vartheta) = \pm\sinh\vartheta, \quad f(\vartheta) = \pm\cosh\vartheta.$$

For some solutions their Taylor expansions were found and other ones are given in the tables.[15]

It is worth noting,[19] that all the second-order ODE's

$$\frac{d^2\vartheta}{du^2} = F\left(\frac{d\vartheta}{du}, \vartheta, u\right)$$

(where F is rational in ϑ and in $d\vartheta/du$ and analytic in u) without movable critical points are reduced [by some homographic transformation $\vartheta = (l(s)w + m(s))/(p(s)w + q(s))$ and exchanging the variables $u = \phi(s)$] either to Riccati equations or to elliptic functions or one of the following six types of Painlevé transcendents[20]:

$$P_1: \frac{d^2\vartheta}{du^2} = 6\vartheta^2 + u,$$

$$P_2: \frac{d^2\vartheta}{du^2} = 2\vartheta^3 + u\vartheta + \alpha,$$

$$P_3: \frac{d^2\vartheta}{du^2} = \frac{1}{\vartheta}\left(\frac{d\vartheta}{du}\right)^2 - \frac{1}{u}\frac{d\vartheta}{du} + \frac{1}{u}(\alpha\vartheta^2 + \beta) + \gamma\vartheta^3 + \frac{\sigma}{\vartheta},$$

$$P_4: \frac{d^2\vartheta}{du^2} = \frac{1}{2\vartheta}\left(\frac{d\vartheta}{du}\right)^2 + \frac{3\vartheta^3}{2} + 4u\vartheta^2 + 2(u^2 - \alpha)\vartheta + \frac{\beta}{\vartheta},$$

$$P_5: \frac{d^2\vartheta}{du^2} = \left\{\frac{1}{2\vartheta} + \frac{1}{\vartheta - 1}\right\}\left(\frac{d\vartheta}{du}\right)^2 - \frac{1}{u}\frac{d\vartheta}{du} + \frac{(\vartheta-1)^2}{u^2}\left\{\alpha\vartheta + \frac{\beta}{\vartheta}\right\}\frac{\gamma\vartheta}{u} + \frac{\sigma\vartheta(\vartheta+1)}{\vartheta - 1}.$$

$$P_6: \frac{d^2\vartheta}{du^2} = \frac{1}{2}\left\{\frac{1}{\vartheta} + \frac{1}{\vartheta - 1} + \frac{1}{\vartheta - u}\right\}\left(\frac{d\vartheta}{du}\right)^2 - \left\{\frac{1}{u} + \frac{1}{u-1} + \frac{1}{\vartheta - u}\right\}\frac{d\vartheta}{du} + \frac{\vartheta(\vartheta-1)(\vartheta-u)}{u^2(u-1)^2} \times\left\{\alpha + \frac{\beta u}{\vartheta^2} + \frac{\gamma(u-1)}{(\vartheta-1)^2} + \frac{\sigma u(u-1)}{(\vartheta-u)^2}\right\}.$$

In some cases this fact is very helpful when looking for the solutions of Eqs. (6.2a) and (6.3) in a closed form. Now we shall give the solutions of Eq. (6.1) for a few special forms of f.

A. The polynomial d'Alembert equation

Let

$$f(\vartheta) = 4A\vartheta^3 + 3B\vartheta^2 + 2C\vartheta + D, \quad A,B,C,D, \in \mathbb{R}^1. \tag{6.4}$$

From Eq. (6.2a) we have

$$\tfrac{1}{2}\vartheta'^2 = A\vartheta^4 + B\vartheta^3 + C\vartheta^2 + D\vartheta + E, \quad E \in \mathbb{R}^1, \tag{6.5}$$

where E is the constant of integrability. Now we present the procedure of construction of the general solution of this equation. It can be expressed by the Weierstrass P-function[20,21] satisfying the equation

$$P'^2 = 4P^3 - g_2P - g_3. \tag{6.6}$$

The so-called invariants g_2 and g_3 are homogeneous functions of the periods ω_1, ω_2 of the -4th- and -6th-order, respectively, and are given by the formulas

$$g_2(\omega_1,\omega_2) = 60\sum_{m,m'}{}' \frac{1}{(m\omega_1 + m'\omega_2)^4},$$
$$g_3(\omega_1,\omega_2) = 140\sum_{m,m'}{}' \frac{1}{(m\omega_1 + m'\omega_2)^6}. \tag{6.7}$$

In our case the values of the invariants g_2 and g_3 are given by

$$g_2(\omega_1, \omega_2) = a_4 - 4a_1a_3 + 3a_3 =: q, \tag{6.8}$$

$$g_3(\omega_1, \omega_2) = \det \begin{vmatrix} 1 & a_1 & a_2 \\ a_1 & a_2 & a_3 \\ a_2 & a_3 & a_4 \end{vmatrix} =: p,$$

where

$$a_1 := \frac{B}{2\sqrt{2A}}, \quad a_2 := \frac{C}{3}, \quad a_3 := D\sqrt{\frac{A}{2}}, \quad a_4 := 4AE.$$

The existence of periods ω_1 and ω_2 guarantees the following fact.[21] For every real number c, the equation $J(\tau) = c$ [where $J(\tau) = g_2^3/(g_2^3 - 27g_3^2)$ is the module function of $\tau := \omega_1/\omega_2$] possesses exactly one root in the fundamental region of the modular group. Thus, taking $c := q^2/(q^3 - 27p^2)$ we can obtain the ratio $\tau = \omega_1/\omega_2$. If $g_2 = q \neq 0$ then from the homogenity of the function g_2 we can determine

$$\omega_1^4 = q^{-1} \cdot g_2(1, \tau),$$

and, when $g_2 = q = 0$ we have

$$\omega_1^6 = p^{-1} \cdot g_3(1, \tau).$$

When ω_1 is found, then ω_2 is determined from the formula $\omega_2 = \tau^{-1}\omega_1$, and ω_1 and ω_2 calculated in such a way satisfy (6.8). It is well known that one can uniquely determine a quantity t satisfying the system

$$P(t, \omega_1, \omega_2) = a_1^2 - a_2,$$

$$P'(t, \omega_1, \omega_2) = 2a_1^3 + a_3 - 3a_1a_2.$$

For such t the solution of Eq. (6.5) can be written in the following form[22]:

$$\vartheta(u) = (2A)^{-1/2} g(u, t), \tag{6.9}$$

where the function g is given by formula

$$g(u, t) = \frac{1}{2} \cdot \frac{P'(u + t/2, \omega_1, \omega_2) + P'(u - t/2, \omega_1, \omega_2)}{P(u + t/2, \omega_1, \omega_2) - P(u - t/2, \omega_1, \omega_2)} - a_1.$$

It may happen that one of the periods (say ω_2) becomes infinite, $\omega_2 = \infty$; it takes place when $g_2^3 - 27g_3^2 = 0$. In this case we can express the solution by trigonometric functions, using the formula

$$P(u, \omega_1, \infty) = -\frac{1}{3}\left(\frac{\pi}{\omega_1}\right)^2 \frac{1}{\sin(2\pi \cdot u/\omega_1)},$$

where

$$\omega_1 = \pi(2g_2/9g_3)^{1/2}.$$

By specification of the right-hand side of Eq. (6.4) we get particular equations appearing in various branches of mathematical physics. For many special cases we can find explicit solutions in a closed form. For example, let us consider the equations of motion for the massive SU(2) Yang–Mills theory

$$\partial^\nu G^a_{\mu\nu} = e\epsilon_{abc} G^b_{\mu\nu} W^\nu_c + \mu^2 W^a_\mu,$$

where

$$G^a_{\mu\nu} = \partial_\mu W^a_\nu - \partial_\nu W^a_\mu + e\epsilon_{abc} W^b_\mu W^c_\nu.$$

By the so-called t'Hooft–Coorigan–Fairlie–Wilczek ansatz

$$eW^a_0 = i\frac{\partial v/\partial x^a}{v}, \quad eW^a_i = \epsilon_{ain}\frac{\partial v/\partial x^n}{v} + i\delta_{ai}\frac{\partial v/\partial x^0}{v},$$

the potential W^a_μ may be reduced to a potential satisfying the scalar Φ^4-theory equation[23]

$$\Box v - \tfrac{1}{2}\mu^2 v + \lambda v^3 = 0, \quad \mu, \lambda \in \mathbb{R}^1. \tag{6.10}$$

In our case the ordinary equation (6.5) can be reduced by a particular choice of constants $A = -\lambda/4$, $C = \mu^2/4$, $B = D = 0$ to the elliptic equation which may be solved using the Jacobi function.[20,22] So we obtain[24,25]

$$\begin{aligned} \vartheta(u) &= \vartheta_0 \cdot \mathrm{sn}(A_1 u + E_1, k_1), \\ \vartheta(u) &= \vartheta_0 \cdot \mathrm{cn}(A_2 u + E_2, k_2), \\ \vartheta(u) &= \vartheta_0 \cdot \mathrm{dn}(A_3 u + E_3, k_3), \end{aligned} \tag{6.11}$$

where the Jacobi parameters k_i are given by

$$k_1^2 = \frac{-\lambda\vartheta_0^2}{2A_1^2}, \quad A_1^2 = -\frac{\mu^2}{2} + \frac{\lambda}{2}\vartheta_0^2,$$

$$k_2^2 = \frac{\lambda\vartheta_0^2}{4A_2^2}, \quad A_2^2 = -\frac{\mu^2}{2} + \lambda\vartheta_0^2.$$

$$k_3^2 = k_1^{-2}, \quad A_3^2 = \frac{\lambda\vartheta_0}{2}.$$

In this particular case the solutions can be interpreted as "periodic waves" (periodic potential).

Let us consider a particular d'Alembert equation of the form

$$\Box v = \mu v + v^n,$$

that is, $f(\vartheta) = \mu\vartheta + \vartheta^n$. In our case the ODE (6.2a) can be reduced to the elliptic equation

$$\vartheta' = \pm\{[2/(n+1)]\vartheta^{n+1} + \mu\vartheta^2 + E\}^{1/2}, \quad E \in \mathbb{R}^1.$$

For example when $n = 2$ the solution of this equation can be expressed by the Weierstrass P-function satisfying Eq. (6.6). In this case the invariants g_2 and g_3 are given by

$$g_2(\omega_1, \omega_2) = \frac{\mu}{12}, \quad g_3(\omega_1, \omega_2) = -\left(\frac{\mu}{6}\right)^3 + \frac{E}{36}.$$

If the periods ω_1, ω_2 are obtained then the solution of the ODE (6.2a) takes the form

$$\vartheta = 6P(u, \omega_1, \omega_2) - \mu/2.$$

Let us consider the second situation when the function (6.4) is inserted into Eq. (6.3). If A, B, C, D satisfy the condition

$$D = \frac{B^3}{(4A)^2} + \frac{B(4A)^{2/3} \cdot (8AC - 3B^2)}{4A},$$

then the substitution $\vartheta = (y - B(4A)^{-2/3})/\sqrt[3]{4} \cdot B$ gives

$$y''(s) + ((r-1)/s)\, y'(s) \pm 2(\mu y(s) + \lambda y(s)^3) = 0,$$

where $\mu := (4A)^{-2/3}(8AC - 3B^2)$, $\lambda := (4A)^{1/3}$. It is known[18] that if $r = 3$ then the above equation has a unique solution $y = y(s)$ which is of class C^2 on $(0, \infty)$ and satisfies the conditions

$$\lim_{s\to 0} y(s) = \text{const} > 0, \quad \lim_{s\to 0} y'(s) = 0, \quad \lim_{s\to\infty} y(s) = 0.$$

Let $f(\vartheta) = \mu\vartheta + \lambda\vartheta^5$, where $\mu < 0, \lambda < 0$. If $r = 3$ then the solution of the ODE (6.3) obtained by the Kurdgelaidze techniques takes the form[24]

$$\vartheta = ((\lambda/\beta)^{1/4} s_0)^{-1/2} (s/s_0)^{1/2} Z\{\omega(s/s_0)\},$$

where $Z(\omega)$ is a solution of the equation

$$Z_\omega^2 + \alpha Z^2 + (\beta/3) Z^6 = C_1$$

and

$$\omega(s/s_0) = (\lambda/\beta)^{1/4} \ln(s/s_0)$$

where C_1, s_0, α and β are real constants. In general $Z(\omega)$ can be expressed by elliptic functions.[20] In particular case when $C_1 = 0$ the solution takes the form (Schonster–Emden[15])

$$\vartheta = (3/s_0)^{1/4} (1 + (s/s_0)^2)^{-1/2}.$$

Let us consider the special situation when the function $f(\vartheta) = \lambda \vartheta^n$ is inserted into Eq. (6.3). If $r = 2(n+2)/(n+1)$ then the solution of the ODE (6.3) obtained by Kurdgelaidze techniques takes the form

$$\vartheta(s) = (\beta C_1^2/\lambda)^{1/n+3} (s/s_0)^{-2/n+1} Z[\omega(s)], \quad s_0, C_1 \in \mathbb{R}^1, \tag{6.12}$$

where $Z(\omega)$ is a solution of the Emden–Fauler equation

$$Z_\omega^2 + \frac{2\beta}{n+1} Z^{n+1} = C_2, \quad Z_\omega = \frac{dZ}{d\omega}, \quad C_2, \beta \in \mathbb{R} \tag{6.13}$$

and

$$\omega(s) = C_1 \left(\frac{\lambda}{\beta C^2}\right)^{2/n+3} s_0 \int_1^{s/s_0} \left(\frac{s}{s_0}\right)^{-(n-1)/(n+1)} d\left(\frac{s}{s_0}\right).$$

If $C_2 = 0$ then we can find a special class of solutions of Eq. (6.13). Hence we have

$$\vartheta(s) = \left(\frac{\beta C_1^2}{\lambda}\right)^{1/n+3} \left(\frac{s}{s_0}\right)^{-2/n+1} \left(\frac{2(n+1)}{\beta(n-1)^2}\right)^{1/n-1} \cdot \left\{ C_1 \left(\frac{\lambda}{\beta C_1^2}\right)^{2/n+3} s_0 \int_1^{s/s_0} \left(\frac{s}{s_0}\right)^{-(n-1)/(n+1)} \times d\left(\frac{s}{s_0}\right) \right\}^{2/1-n}.$$

In the particular case for $f(\vartheta) = \lambda \vartheta^3$, where $\lambda < 0$ and $r = 4$, the ODE (6.3) may be solved using a Jacobi function, so we obtain[24]

$$\vartheta(s) = \sqrt{\frac{2k^2}{\lambda s_0^2 (2k^2 - 1)}} \left(\frac{s_0}{s}\right)^{1/2} \mathrm{Cn}\left\{ \frac{1}{\sqrt{2k^2 - 1}} \ln \frac{s}{s_0} \right\},$$

where s_0 is an arbitrary constant and k is the Jacobi parameter. If $\frac{1}{2} < k^2 < 1$ then the solution describes periodic oscillation with vanishing amplitude. When $k^2 = 1$ the periodic oscillations transform into hyperbolic oscillations. Hence we obtain

$$\vartheta(s) = 2\sqrt{\frac{2}{\lambda s_0^2}} \frac{(s/s_0)}{1 + (s/s_0)^2}.$$

B. The Liouville equation

The Liouville equation we obtain taking, in (6.1), $f(\vartheta) = \mu \exp(\vartheta)$. In the two-dimensional case, $n = 2$, the general solution of (6.1) is well known[26]:

$$v = \ln\left(\frac{8}{|\mu|} \cdot \frac{f'(x+t) \cdot g'(x-t)}{[f(x+t) - g(x-t)]^2} \right)$$

(f and g are arbitrary functions of one variable). It may be simply obtained using our method. For many dimensions our procedure gives for the solution of Eq. (6.2a) the following expression:

$$\vartheta(u) = \ln(P(\pm(\sqrt{\mu/2})u, \omega_1, \omega_2) - (1/3\mu)D), \quad D \in \mathbb{R}^1, \tag{6.14}$$

where P is the P–Weierstrass function with the invariants g_2 and g_3 given in the form

$$g_2(\omega_1, \omega_2) = 4D^2/3\mu^2, \quad g_3(\omega_1, \omega_2) = 8D^3/27\mu^3. \tag{6.15}$$

Some people[27] think that in quantum field theory particles are described as the singular solutions of the Liouville equation. The solution (6.14) with u as in (3.2a) describes the movement of a single particle in the Euclidean quantum field theory.

Another application of the Liouville equation is in plasma physics. Let us consider electrical potential v created by particle distribution (ions, electrons, etc., with charge Z_e, e the elementary charge, Z a nonzero, integer number) at absolute temperature T. Let the concentration of charged particles be n_0. Then we have the following equation[28] for potential v_1:

$$\Delta v_1 = -4\pi e n_0 \exp(-Z e v_1/kT).$$

By substituting $v = -Z e v_1/kT$ we obtain the right-hand side of the form $f(v) = \mu \exp v$, where $\mu = 4\pi e^2 n_0/kT$. The obtained solution (6.14), where u is given by (3.2a), describes self-consistent potential created by charged particles at temperature T. This potential always has a singular point, given by the equation

$$P(\pm(\sqrt{\mu/2})u, \omega_1, \omega_2) - (1/3\mu) D = 0.$$

Therefore we can consider this solution as a logarithmic potential created by an effective point charge located at a singular point.

In turn, substituting $f(\vartheta) = \mu \exp$ in Eq. (6.2b) gives

$$2u\vartheta'' + r\vartheta' = \mu \exp \vartheta.$$

By substituting $\vartheta = \ln \Psi$, it can be reduced to

$$\ddot{\Psi} - \frac{\dot{\Psi}}{\Psi} + \frac{r}{2s}\dot{\Psi} - \frac{\mu}{s}\Psi^2 = 0,$$

where $\dot{\Psi} := d\Psi/ds$, $s = u/2$.

For $r = 2$ the above equation becomes[20] the third equation of the Painlevé P_3 type for an unknown function Ψ.

C. The sine–Gordon equation

Let us consider now the sine–Gordon equation [ie., $f(\vartheta) = \sin \vartheta$].

We start with Eq. (6.2a). Substituting $\vartheta = 4 \arctan \Psi$ for the sine–Gordon equation gives

$$\Psi'^2 = \frac{D-1}{8}\Psi^4 + \frac{D+3}{4}\Psi^2 + \frac{D-1}{8}, \quad D \in \mathbb{R}^1,$$

where D is the constant of integrability. This ODE is of the form (6.5) and the method described in Sec. VI A may be used, giving for Ψ the same expressions as in (6.9) for ϑ.

In turn, Eq. (6.2b), after the substitution $\vartheta = -i \ln \Psi$ for the sine–Gordon equation gives

$$\Psi'' - \frac{\Psi'^2}{\Psi} + \frac{r}{2u}\Psi' - \frac{1}{4u}\Psi^2 + \frac{1}{4u} = 0. \qquad (6.16)$$

The condition of reality ϑ requires that $|\Psi| = 1$. For $r = 2$, Eq. (6.16) becomes the third equation of the Painlevé P_3 type. There is also another possible way. Namely inserting $\vartheta = \epsilon\Psi^2$ with $\epsilon = \pm 1$ into equation (6.2b) we obtain

$$\ddot{\Psi} = \left(\frac{1}{2\Psi} + \frac{1}{1+\Psi}\right)\dot{\Psi}^2 - \frac{r-1}{s}\dot{\Psi} + \frac{8\Psi(1-\Psi)}{1+\Psi}$$

if $\epsilon = 1$, and

$$\ddot{\Psi} = -\left(\frac{1}{2\Psi} - \frac{1}{1-\Psi}\right)\dot{\Psi}^2 + \frac{r-1}{s}\dot{\Psi} + \frac{8\Psi(1+\Psi)}{\Psi-1}$$

if $\epsilon = -1$, where $\dot{\Psi} := d\Psi/ds$, $s = |u|^{1/2}$. This equation is of the Painlevé P_5 type.[20]

D. The cosh- and sinh-d'Alembert equations

Let us consider the d'Alembert equation (6.1) with the right-hand side of the hyperbolic type:

(a) $f(\vartheta) = \cosh\vartheta$ and (b) $f(\vartheta) = \sinh\vartheta$.

By substituting $\vartheta = 4 \operatorname{arctanh}\Psi$ the ODE (6.2a) leads to the equation

$$\Psi'^2 = \tfrac{1}{2}\Psi(1+\Psi^2) + (C/8)(1-\Psi^2)^2$$

for the case (a), and

$$\Psi'^2 = \Psi^2 + (C + 1/8)(1-\Psi^2)^2$$

for the case (b), where C is the integral constant. Both these equations are of the considered form (6.5). If in particular $C = 0$ then we obtain the following solutions:

$$\vartheta(u) = \ln(4P(u\,\omega_1, \omega_2) - \tfrac{2}{3}D),\ D \in \mathbb{R}^1, \qquad (6.17)$$

where P is the P–Weierstrass function with the invariants g_2 and g_3 given, respectively, by the formulas

$$g_2(\omega_1, \omega_2) = \tfrac{1}{4}(\tfrac{4}{3}D^2 \pm 1), \quad g_3(\omega_1, \omega_2) = -D(D^2/27 \pm \tfrac{1}{24}),$$

where the upper sign refers to the case (a) and the lower to the case (b).

In turn Eq. (6.2b), after substituting $\vartheta = \ln\Psi$, gives

$$\Psi'' - \frac{\Psi'^2}{\Psi} + \frac{r}{2u}\Psi - \frac{1}{4u}\Psi^2 \mp \frac{1}{4u} = 0,$$

where the upper and the lower signs refer to the case (a) and (b), respectively. This is a Painlevé P_3 type equation.

ACKNOWLEDGMENTS

We are greatly indebted to Professor R. Raczka and Professor R. Zelazny for very inspiring discussions during the study of the subject.

This work was partially supported by the National Science Foundation under Grant No. INT 73-20002, A-01 formerly GF-41958.

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Hamiltonians with high-order integrals and the "weak-Painlevé" concept

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(Received 22 February 1984; accepted for publication 1 June 1984)

We examine the singularity structure of the equations of motion associated to integrable two-dimensional Hamiltonians with second integrals of order higher than 2. We show in these specific examples that the integrability is associated to a singularity expansion of the "weak-Painlevé" type. New cases of integrability are discovered, with still higher-order integrals which are explicitly computed.

PACS numbers: 03.20. + i, 02.30. + g

I. INTRODUCTION

The singularity analysis is a most useful tool in the study of nonlinear dynamical systems. The interest in this method has been kindled by the conjecture of Ablowitz, Ramani, and Segur (ARS)[1] who related integrability to the singularity structure through the Painlevé property. The latter is associated to the absence of critical movable singularities on the complex time plane, i.e., the singularities of the solutions are simply poles. The power of the ARS conjecture has been amply demonstrated by various works where it was shown that well-known integrable systems pass the Painlevé test. However, and what is more important, this approach has made possible the identification of new classes of integrable systems.[2]

In a recent work we have examined the possibility of integrability existing independently of the Painlevé property. We thus discovered two-dimensional polynomial Hamiltonians which possess a second integral of motion, and where the equations of motion were not of the Painlevé type. However they possess movable singularities of particularly simple algebraic-cut form $(t - t_0)^{1/n}$. Such a behavior was dubbed the "weak-Painlevé" property and has been extremely useful in producing 2-D integrable Hamiltonians.[3]

Once the "weakened" version of the Painlevé conjecture was proposed, two important questions have been asked by Kruskal and Fokas. Kruskal's question was whether the full-Painlevé property (pure pole behavior) could not be recovered from the weak Painlevé one with an adequate change of variables. This question has been dealt with in detail in a previous article.[4] We have shown that the two-dimensional Hamiltonian systems exhibiting the weak-Painlevé behavior, and which are associated to constants of motion quadratic in the velocities, are separable in some sense. The equations for the trajectory indeed separate when one expresses them in the adequate coordinate system.[5] Our analysis has shown that the equations of motion, even when expressed in the coordinate system which lead to separation, still are of "weak" rather than the full-Painlevé type. Fokas' remark at this point was that a genuine test of the weak-Painlevé criterion would be offered by integrable Hamiltonians which are decidedly nonseparable. Therefore 2-D Hamiltonians with a second integral of degree higher than 2 in the velocities were investigated.

The aim of this paper is to examine, from the point of view of the singularity structure, two Hamiltonians: one due to Fokas himself[6] and one due to Holt,[7] for which cubic integrals of motion are known. We will show that these Hamiltonians lead indeed to expansions of the weak-Painlevé type for the solutions. In the case of the Holt Hamiltonian, further cases of integrability are discovered. Their second integrals are calculated. In the process of calculating these integrals we investigate the possibility of modifying the potential through additional terms while preserving integrability. We derive thus the additive terms for the Holt potential and for the Hénon–Heiles one (which we have analyzed in a previous work[8]).

II. PAINLEVÉ ANALYSIS OF THE FOKAS–LAGERSTROM HAMILTONIAN

In a recent paper,[6] Fokas and Lagerstrom proposed the two-dimensional integrable Hamiltonian

$$H = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) + (x^2 - y^2)^{-2/3}, \tag{1}$$

for which the second integral is

$$I = (\dot{x}^2 - \dot{y}^2)(x\dot{y} - y\dot{x}) - 4(y\dot{x} + x\dot{y})(x^2 - y^2)^{-2/3}. \tag{2}$$

The Hamiltonian assumes an even simpler expression in the variables $x \pm y$.

We rewrite H, up to scalings, as

$$H = \tfrac{1}{2}(\dot{X}^2 + \dot{Y}^2) + \tfrac{3}{2}(XY)^{-2/3}. \tag{3}$$

The equations of motion read

$$\ddot{X} = X^{-5/3}Y^{-2/3}, \quad \ddot{Y} = X^{-2/3}Y^{-5/3}. \tag{4}$$

An obvious possible singular behavior is

$$X \sim Y \sim (t - t_0)^{\alpha},$$

with $\alpha - 2 = -\frac{7}{3}\alpha$, i.e., $\alpha = \frac{3}{5}$.

The leading behavior is not a pole. *A priori*, one could expect either of two possibilities: the full-Painlevé situation, where X^5 and Y^5 have a pure triple pole; or the weak-Painlevé case, where all powers of $(t - t_0)^{1/5}$ appear in the expansion.

In order to settle this question, we compute the resonances.[1] We find -1, $-\frac{4}{5}$, $\frac{3}{5}$, and $\frac{4}{5}$. As usual, -1 is associated to the arbitrariness of t_0 and two free parameters enter at

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order $\frac{3}{5}$ and $\frac{4}{5}$. We are thus in a weak-Painlevé situation.

Because of the presence of one negative resonance besides -1, this solution depends on three free parameters instead of four, and is not generic. We must now look for the generic singular solution. Up to the exchange of x and y, this solution is obtained when Y has a divergent second derivative, but has a finite, nonzero limit A at the singularity.

The dominant part of the X equation is

$$\ddot{X} = A^{-2/3} X^{-5/3},$$

giving the leading behavior $X \sim (t - t_0)^{3/4}$ and resonances -1 and $+\frac{1}{2}$ (this is still a weak-Painlevé situation).

As for Y it behaves as

$$Y = A + B(t - t_0) + C(t - t_0)^{3/2} + \cdots,$$

with A and B free. The $(t - t_0)^{3/2}$ term in Y is such that its second derivative balances the most divergent term (proportional to $X^{-2/3}$) in the corresponding equation.

The four free parameters of this generic solution are t_0, A, B, and the coefficient of $(t - t_0)^{5/4}$ in X [or, equivalently, of $(t - t_0)^2$ in Y] which is related to the energy.

In conclusion, both the obvious, nongeneric solution and the (far from obvious) generic one have weak-Painlevé type expansions. This would suffice in order to answer Fokas' question as to the existence of nonseparable potentials with the weak-Painlevé property. However, further examples can be offered.

III. PAINLEVÉ ANALYSIS OF THE HOLT HAMILTONIANS

In his analysis of integrable potentials in two dimensions, Holt has constructed a Hamiltonian which possesses a second integral cubic in the velocities.[7,9] The form of this Hamiltonian is

$$H = \tfrac{1}{2}(\dot{x}^2 + \dot{y}^2) - \tfrac{3}{4}\lambda x^{4/3} - (y^2 - \tfrac{3}{2}\mu)x^{-2/3}, \tag{5}$$

with $\lambda = 1$ (we have introduced λ for further use).

Its second integral, still for $\lambda = 1$, reads

$$C = \dot{y}(2\dot{y}^2 + 3\dot{y}\dot{x}) - 3\dot{y}[2(y^2 - \tfrac{3}{2}\mu)x^{-2/3} - 3x^{4/3}] - 18\dot{x}yx^{1/3}. \tag{6}$$

The corresponding equations of motion are

$$\ddot{x} = \lambda x^{1/3} + \mu x^{-5/3} - \tfrac{2}{3}y^2 x^{-5/3}, \quad \ddot{y} = 2yx^{-2/3}. \tag{7}$$

The Painlevé analysis in the case $\mu \neq 0$ is quite intricate. In fact it resembles closely the analysis we presented for Fokas' Hamiltonian. That is, y has a divergent second derivative but a finite nonzero limit at the singularity.

Three cases can be distinguished (in which the parameter λ does not play any role).

(i) $x \sim A\tau^{6/5}$, $y \sim \sqrt{\frac{3\mu}{2}} + B\tau^{6/5}$ $(\tau = t - t_0)$,

where A, B are determined by the most diverging term in the equations of motion. The resonances in this case are -1, $-\frac{4}{5}$, $-\frac{3}{5}$, $-\frac{2}{5}$. So this is a one-parameter solution.

(ii) $x \sim A\tau^{9/8}$, $y \sim \sqrt{\frac{3\mu}{2}} + B\tau + C\tau^{5/4}$,

where one free parameter, say B, determines A and C. We look for the resonances through a term $\gamma\tau^{5/4+n}$ in y. We find $n = -\frac{5}{4}$ which means that t_0 is free, $n = -\frac{1}{4}$ (B is free) and $n = -\frac{1}{2}$, $-\frac{3}{4}$, which are just formal resonances. This is a two-parameter solution.

(iii) $x \sim D\tau^{3/4}$, $y \sim A + B\tau + C\tau^{3/2}$,

with A and B free (C and D fixed through Eq. 7). We look for resonances through terms $\gamma\tau^{3/4+n}$ in x and $\delta\tau^{3/2+n}$ in y. We find $n = -1$ (due to t_0), $n = -\frac{3}{2}$, $-\frac{1}{2}$ (associated to A and B), and $n = \frac{1}{2}$ which is a genuine resonance (related to the energy). So the solution is the generic four-parameter one and it is of the weak-Painlevé type.

We now turn to the case $\mu = 0$, for which λ will play an essential role. In this case x diverges as $x \sim \tau^3$ while y can diverge either as $y \sim \tau^3$ or as $y \sim \tau^n$ with rational n.

In the first case ($y \sim \tau^3$) the resonance condition leads to

$$6\lambda = 6 + m(m + 1), \tag{8}$$

where m must be an integer. In the second case ($y \sim \tau^n$) we obtain

$$n(n - 1) = 12/\lambda. \tag{9}$$

The only rational solutions to systems (8), (9) are

$$\lambda = 1, \quad m = 0, \quad n = 4,$$
$$\lambda = 2, \quad m = 2, \quad n = 3,$$
$$\lambda = 6, \quad m = 5, \quad n = 2,$$
$$\lambda = 16, \quad m = 9, \quad n = \tfrac{3}{2},$$
$$\lambda = 27, \quad m = 12, \quad n = \tfrac{4}{3},$$
$$\lambda = \tfrac{256}{3}, \quad m = 22, \quad n = \tfrac{9}{8}.$$

Of these solutions $\lambda = 1$ corresponds to the known Holt potential; $\lambda = 2$ is a formal solution of (8), (9) which does not satisfy the Painlevé property. Indeed, the leading behavior is not rational but logarithmic. Cases $\lambda = 6$, $\lambda = 16$ are new integrable cases which possess the full Painlevé property (for $\lambda = 16$ this is true in terms of y^2 rather than y). We have indeed been able to compute the integrals of motion of these two cases at order 4 and 6 in the velocities. The two remaining cases are, at best, genuine weak-Painlevé cases and candidates for integrability. However we have not been able to identify a second constant of motion, at least up to order 6 in the velocities.

IV. DIRECT SEARCH FOR INTEGRALS OF MOTION FOR THE HOLT POTENTIAL

In this section, we look for potentials of the form

$$V = y^2 G_1''(x) + yG_2'(x) + G_3(x) + F(y), \tag{10}$$

for which the equations of motion admit, apart from the energy, a second invariant quartic in the velocities. Such potentials are a generalization of Holt's form. Following the method exposed in Refs. 2 and 8, one immediately sees that because

$$V_{xy^3} = 0,$$

the form of the invariant will be

$$C = f_0\dot{x}^4 + g_0\dot{x}^2 + g_1\dot{x}\dot{y} + g_2\dot{y}^2 + h, \tag{11}$$

where f_0 is a constant and g_0, g_1, g_2, h are functions of x and y.

The expressions for the g_i's read

$$g_0 = y^2 G_1'' + yG_2' + G_3, \quad g_1 = -2yG_1' - G_2,$$
$$g_2 = 2G_1 \quad (\text{with } 4f_0 \equiv 1). \tag{12}$$

We now write the last relation that allows the calculation of h and which will impose constraints on the nature of the arbitrary functions G_i and F:

$$g_1(V_{xx} - V_{yy}) + 2(g_2 - g_0)V_{xy} - (2g_{0,y} - g_{1,x})V_x + (2g_{2,x} - g_{1,y})V_y = 0. \tag{13}$$

It is clear that different kinds of terms will be involved in this relation.

Let us first consider the case where $F = 0$; the only terms depending on y in this relation are of the form $y^k \varphi(x)$, for k a non-negative integer up to 3.

The preceding relation leads thus to four distinct equations. Quite easily, one realizes that G_2 has to be set to zero if $G_1''' \neq 0$ and we are thus left with the two relations

$$G_1' G_1'''' + 5G_1'' G_1''' = 0, \quad G_1' J'' + 3G_1'' J' + 2G_1''' J = 0 \quad (\text{with } J = G_3 - 2G_1). \tag{14}$$

A nice algebraic solution (with $G_1'' \neq 0$) is

$$G_1 = \tfrac{9}{4}x^{4/3}.$$

Integration for J is quite easy and reads

$$J = \kappa x^{2/3} + \mu x^{-2/3},$$

and the potential V has the form

$$V = x^{-2/3}y^2 + \kappa x^{+2/3} + \mu x^{-2/3} + \tfrac{9}{2}x^{4/3}. \tag{15}$$

We will now introduce the function F. If F is not polynomial, it will not interfere with other terms in relation (13). Thus G_1 and J are not modified, which leads to the following equation for F:

$$3F' + yF'' = 0,$$

that is, $F = \nu/y^2$.

The most general solution of that kind is thus the following:

$$V = x^{-2/3}y^2 + \kappa x^{2/3} + \mu x^{-2/3} + \tfrac{9}{2}x^{4/3} + \nu/y^2. \tag{16}$$

This is in fact a generalization of the Holt potential with $\lambda = 6$ which we recover for $\kappa = \nu = 0$. However we have two extra terms in $x^{2/3}$ and $1/y^2$ which are compatible with the existence of an integral of order 4:

$$C = \dot{x}^4/4 + (y^2 x^{-2/3} + \kappa x^{2/3} + \tfrac{9}{2}x^{4/3} + \mu x^{-2/3})\dot{x}^2 - 6x^{1/3}y\dot{x}\dot{y} + \tfrac{9}{2}x^{4/3}\dot{y}^2 + y^4 x^{-4/3} - 9y^2 x^{2/3} - 2\kappa y^2 + \kappa^2 x^{4/3} + 9\kappa x^2 + \tfrac{81}{4}x^{8/3} + 2y^2\mu x^{-4/3} + 9\mu x^{2/3} + \mu^2 x^{-4/3} + 9\nu x^{4/3}y^{-2}. \tag{17}$$

At this point two interesting results can be obtained concerning previously studied Hamiltonians. Indeed consider the case where F is a polynomial of degree 4, namely

$$F' = ay^3 + by^2 + cy + d.$$

Consider first solutions where $G_2 = 0$.

The two preceding relations for G_1 and J are transformed into

$$G_1' G_1 + 5G_1'' G_1 - 6aG_1' = 0,$$

$$G_1' J'' + 2G_1''' J + 3G_1'' J' - 4cG_1' = 0,$$

and $b = d = 0$.

From the first equation, we get

$$G_1 = (\lambda/4)x^4, \; a = 16\lambda,$$

from which one obtains for J,

$$J = \kappa x^2 + \mu x^{-2} + \nu x^{-6},$$

and the solution V writes

$$V = 8y^4 + 6x^2y^2 + x^4 + \mu x^{-2} + \nu x^{-6} + \kappa(x^2 + 4y^2). \tag{18}$$

This potential has been examined in our paper on integrable polynomial potentials, and its second integral of motion was identified. We remark here that the additional terms $\mu x^{-2} + \nu x^{-6}$ do not destroy integrability. Indeed the second integral is

$$C = \dot{x}^4 + (24x^2y^2 + 4x^4 + 4\nu x^{-6} + 4\mu x^{-2} + 4\kappa(x^2 + 4y^2))\dot{x}^2 - 16yx^3\dot{x}\dot{y} + 4x^4\dot{y}^2 + 16x^4y^4 + 16x^6y^2 + 4x^8 + 16\kappa y^2x^4 + 48\nu x^{-4}y^2 + 16\mu y^2 + 8\kappa x^6 + \frac{8\nu}{x^2} + 4\kappa^2x^4 + \frac{8\kappa\nu}{x^8} + 4\frac{\mu^2 + 2\kappa\nu}{x^4} + 4(\nu^2/x^{12}) + 8\mu x^2. \tag{19}$$

In the case $G_2 \neq 0$, similar calculations lead to the Hénon–Heiles potential which has been integrated by us[10] and, independently, by Hall.[9] The integral of motion is again quartic in the velocities and integrability is preserved despite the addition of terms of the form $\mu/x^2 + \nu/x^6$. So this integrable Hénon–Heiles potential reads

$$V = (a/2)(x^2 + 16y^2) + d(x^2y + \tfrac{16}{3}y^3) + \mu/x^2 + \nu/x^6, \tag{20}$$

with invariant

$$C = \frac{1}{4}\dot{x}^4 + \left[\frac{a}{2}x^2 + dx^2y + \frac{\mu}{x^2} + \frac{\nu}{x^6}\right]\dot{x}^2 - \frac{dx^3}{3}\dot{x}\dot{y} + \frac{2\,d\nu}{x^4}y + \frac{2\mu\nu}{x^8} + \frac{\nu^2}{x^{12}} - \frac{d^2x^4}{3}y^2 - \frac{d^2x^6}{18} + \frac{a^2x^4}{4} + \frac{(a\nu + \mu^2)}{x^4} + \frac{2}{3}\mu\,dy. \tag{21}$$

For the case $\lambda = 16$ we look for a second integral of degree 6 in the velocities (having verified that degree 5 did not lead to any interesting results). We have in general

$$C = e_0\dot{x}^6 + e_1\dot{x}^5\dot{y} + e_2\dot{x}^4\dot{y}^2 + e_3\dot{x}^3\dot{y}^3 + e_4\dot{x}^2\dot{y}^4 + e_5\dot{x}\dot{y}^5 + f_0\dot{x}^4 + f_1\dot{x}^3\dot{y} + f_2\dot{x}^2\dot{y}^2 + f_3\dot{x}\dot{y}^3 + f_4\dot{y}^4 + g_0\dot{x}^2 + g_1\dot{x}\dot{y} + g_2\dot{y}^2 + h, \tag{22}$$

with the f_i's, g_i's, and h functions of x, y and the e_i's constants. The absence of $\dot{y}^6$ in C guarantees that C is not proportional to H^3. From the compatibility conditions[8] we find readily

$$e_3 = e_4 = e_5 = 0,$$

while some further calculations give $e_1 = 0$. The f_i's can thus be computed:

$$f_0 = 6e_0y^2x^\alpha + \tfrac{9}{2}e_0\lambda x^{\alpha+2}, \quad f_1 = 12x^{\alpha+1}y(e_2 - 3e_0),$$
$$f_2 = 4e_2y^2x^\alpha + 9x^{\alpha+2}((\lambda/3)e_2 - e_2 + 3e_0), \tag{23}$$
$$f_3 = -24e_2x^{\alpha+1}y, \quad f_4 = 18e_2x^{\alpha+2},$$

with $\alpha = -\frac{2}{3}$. For the calculation of the g_6's we have a first compatibility condition

$$(\lambda - 21)e_2 + 15e_0 = 0, \tag{24}$$

and their general form is

$$g_0 = A_0 y^4 x^{2\alpha} + B_0 y^2 x^{2\alpha+2} + C_0 x^{2\alpha+4},$$
$$g_1 = A_1 y^3 x^{2\alpha+1} + B_1 y x^{2\alpha+3}, \tag{25}$$
$$g_2 = A_2 y^4 x^{2\alpha} + B_2 y^2 x^{2\alpha+2} + C_2 x^{2\alpha+4},$$

with

$$A_0 = 12e_0, \quad B_0 = 18\lambda e_0 + 36(e_2 - 3e_0), \quad C_0 = \tfrac{27}{4}\lambda^2 e_0,$$
$$A_1 = 24(e_2 - 3e_0), \quad B_1 = \tfrac{26}{5}(e_2 - 3e_0)(4\lambda - 9), \tag{26}$$
$$A_2 = 4e_2, B_2 = 12(\lambda - 6)e_2,$$
$$C_2 = -(e_2 - 3e_0)(\tfrac{351}{4}\lambda - \tfrac{243}{10}) + \tfrac{9}{4}\lambda^2 e_2.$$

The last compatibility relation for the calculation of h reads

$$(e_2 - 3e_0)(\lambda^2 - 7\lambda + 6) = 0. \tag{27}$$

So either $\lambda = 1$ or $\lambda = 6$ or $e_2 = 3e_0$. The first two cases were found previously: for the first, the present invariant is the square of the cubic integral, while for the second, we have the product of the energy times the quartic invariant. The only remaining possibility is $e_2 = 3e_0$ and replacing back into Eq. (24), we find $\lambda = 16$. This gives us a genuine sixth-order integral of motion

$$\begin{aligned} C = {} & \dot{x}^6 + 3\dot{y}^2\dot{x}^4 + 6(\dot{x}^4 + 2\dot{x}^2\dot{y}^2)(y^2 + 12x^2)x^{-2/3} \\ & - 72x^{1/3}y\dot{x}\dot{y}^3 + 54x^{4/3}\dot{y}^4 \\ & + 12(\dot{x}^2 + \dot{y}^2)(y^2 + 144x^4)x^{-4/3} \\ & + 72x^{2/3}y^2(4\dot{x}^2 - 5\dot{y}^2) + 8(y^6 - 35y^4x^2 \\ & + 432y^2x^4 + 1728x^6)x^{-2}. \end{aligned} \tag{28}$$

Cases $\lambda = 27$ and $\lambda = \frac{256}{3}$ do not have second integrals of motion up to degree 6 in the velocities.

V. DISCUSSION AND OUTLOOK

In this paper we have presented evidence that the weak-Painlevé concept which we have introduced in our previous work is not associated exclusively to 2-D Hamiltonians with a quadratic second constant of motion. Two integrable Hamiltonians have been analyzed: one due to Fokas and Lagerstrom and one due to Holt. We have shown that the solutions of both Hamiltonians are of the weak-Painlevé type, i.e., they present algebraic branch points of a specific type fixed by the dominant behavior of the equations of motion. The variety of these "natural" exponents makes the existence of a transformation, through a change of variables, from weak type to a full-Painlevé pole-type expression extremely improbable. (This richness of natural exponents would be even greater if we had included in our Painlevé analysis the additional terms discovered in Sec. IV.)

At this point a question still lingers concerning the Holt potential. Are the cases corresponding to $\lambda = 27$ and $\lambda = \frac{256}{3}$ indeed integrable? (The resonances being at $m = 12$ and $m = 22$, respectively, make the check of the compatibility condition next to impossible.) We have not been able to identify a second constant of motion up to order 6 in the velocities. Calculations beyond this order would necessitate extensive formal computer calculations of increasing complexity.

As a by-product of our calculations we have obtained additional terms for the Hénon–Heiles potential as well as for the quartic polynomial potential, the integrability of which we had treated in our previous work.

As a conclusion we can state once more that the singularity analysis is indeed a most powerful tool in the domain of nonlinear systems.

ACKNOWLEDGMENTS

The authors wish to thank A. Fokas for his remark which was at the origin of this paper. We also wish to thank M. D. Kruskal for stimulating discussions.

Note. Once the present work was completed in its present form, we were informed that J. Hietarinta has performed an analysis of the Holt potential, identifying and integrating the cases $\lambda = 1, 6, 16$ (in our notations). In the latter case he presents a simpler form for the constant by computing $I = H^3 - C$, where C is given by Eq. 28. He finds

$$\begin{aligned} I = {} & \dot{y}^6 + 3\dot{y}^4\dot{x}^2 + (18x^{4/3} + 6y^2x^{-2/3})\dot{y}^4 + 72x^{1/3}y\dot{y}^3\dot{x} \\ & + 648x^{2/3}y^2\dot{y}^2 + 648y^4. \end{aligned}$$

We wish to thank Dr. J. Hietarinta for making his results available to us before publication [J. Hietarinta, Phys. Rev. A **28**, 3670 (1983)].

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Polynomial constants of motion in flat space

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(Received 19 July 1983; accepted for publication 25 April 1984)

Some general results on commuting integrals for a Hamiltonian system are given. The question of the existence of integrals which are polynomial in the momenta is investigated and the results applied to a variety of mechanical systems.

PACS numbers: 03.20. + i, 02.30. + g

I. INTRODUCTION

There seems little need to motivate a paper which is concerned with the existence of explicit integrals of motion in classical mechanics. From the earliest days of the subject much attention has been given to the question of the existence of such integrals; however, comparatively few general results are known. Indeed, at the present time our knowledge is essentially confined to several disparate examples though we do entertain the hope of some much more general unifying theory.

The present paper has several objectives. In Sec. II, I give some results which enable integrals of motion to be written down if the Hamiltonian of the system has a certain form. In Sec. III, I investigate the conditions under which a system has integrals of motion which are polynomial in the momentum variables and make a number of observations about these conditions. In Sec. IV, I work out in detail an example to show how the conditions just referred to may be used in practice and some of the difficulties which may be encountered. In Sec. V several more examples are outlined using the theory of Sec. III.

The notation used here is mainly that of the traditional tensor calculus. The summation convention applies throughout and, with the exception of example (5) in Sec. V, all indices are lowered. The phase space of the systems considered is $2m$-dimensional with m taking particular values in the examples.

II. SOME GENERAL RESULTS ON INTEGRALS OF MOTION

The results which I give here belong properly to the realm of symplectic geometry. Thus, throughout N denotes a symplectic manifold and $\{\ ,\ \}$ denotes the Poisson bracket on $F(N)$, the ring of functions on N.

Proposition 2.1: Suppose that H is the Hamiltonian of a system and that

$$H = f(A,B_1,\ldots,B_r),$$

where $A,B_1,\ldots,B_r \in F(N)$ and f is a function of the $r+1$ arguments indicated. Suppose also that $\{A,B_i\} = 0$ $(1 \leqslant i \leqslant r)$. Then $\{H,A\} = 0$.

The proof of Proposition 2.1 is trivial from the properties of $\{\ ,\ \}$ and though it may seem innocuous it can sometimes yield useful results. The next result has been given before but I shall now expand upon it considerably. Again the proof is straightforward using the derivation properties of $\{\ ,\ \}$.

Proposition 2.2: Suppose that $H,A,B,P,Q \in F(N)$ and that

$$H = (A+B)/(P+Q),$$

where $\{A,B\} = \{P,Q\} = \{A,Q\} = \{P,B\} = 0$. Then

$$\{H,(AQ - BP)/(P+Q)\} = 0.$$

The last result leads immediately to the following, the proof being similar.

Proposition 2.3: Suppose that $H,A_i,P_j \in F(N)$ $(1 \leqslant i,j \leqslant r)$ and that

$$H = (A_1 + A_2 + \cdots + A_r)/(P_1 + P_2 + \cdots + P_r),$$

where

$$\{A_i,A_j\} = \{P_i,P_j\} = \{A_i,P_j\} = 0 \quad (1 \leqslant i,j \leqslant r).$$

Then

$$\frac{A_1(P_2 + \cdots + P_r) - P_1(A_2 + \cdots + A_r)}{P_1 + P_2 + \cdots + P_r},$$

$$\frac{A_2(P_3 + \cdots + P_r + P_1) - P_2(A_3 + \cdots + A_r + A_1)}{P_1 + P_2 + \cdots + P_r},$$

$$\ldots, \frac{A_r(P_1 + \cdots + P_{r-1}) - P_r(A_1 + \cdots + A_{r-1})}{P_1 + P_2 + \cdots + P_r}$$

are r integrals of motion for H which themselves mutually commute. In particular, if $r = \frac{1}{2}\dim(N)$ and these integrals are independent, the system determined by H is completely integrable in the sense of Liouville's theorem.

The last two results seem very closely related to some classical results of Liouville (see Whittaker[1]). Also, one could write down more integrals by using Proposition 2.2 and choosing, for example, $A = A_1 + A_2$, $B = A_3 + \cdots + A_r$, $P = P_1 + P_2$, $Q = P_3 + \cdots + P_r$, etc.

III. CONDITIONS DETERMINING THE EXISTENCE OF POLYNOMIAL INTEGRALS

Consider a standard Hamiltonian of classical mechanics

$$H = \tfrac{1}{2} p_j p_j + V(x_i),$$

where $(x_i, p_j)$is a coordinate system. Suppose that f is a constant of motion for the system determined by H and that

$$f = A_{a_1\cdots a_n} p_{a_1}\cdots p_{a_n} + A_{a_1\cdots a_{n-1}} p_{a_1}\cdots p_{a_{n-1}} + \cdots + A_{a_1} p_{a_1} + A,$$

where $A_{a_1\cdots a_n}, A_{a_1\cdots a_{n-1}}, \ldots, A_{a_1}, A$ are symmetric tensors of

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rank $n, n-1, \ldots, 1, 0$, respectively. The conditions that H and f commute are easily seen to be

$$\begin{aligned} &A_{(a_1 \cdots a_n, a_{n+1})} = 0, \\ &A_{(a_1 \cdots a_{n-1}, a_n)} = 0, \\ &A_{(a_1 \cdots a_{n-2}, a_{n-1})} = nV_{,i} A_{a_1 \cdots a_{n-1} i}, \\ &\vdots \\ &A_{,a_1} = 2V_{,i} A_{a_1 i}, \\ &0 = V_{,i} A_i. \end{aligned} \tag{3.1}$$

Several remarks can be made about (3.1). First, if V is itself a polynomial in coordinates then so too is f. Second, the alternate equations of (3.1) decouple into two sets and so it suffices to look for constants of purely odd and purely even degrees. Third, the first two equations of (3.1) define $A_{a_1 \cdots a_n}$ and $A_{a_1 \cdots a_{n-1}}$ as Killing tensors of the metric δ_{ij} (see Refs. 2 and 3).

A Killing tensor is the natural generalization of a Killing vector which is well known in connection with the existence of momentum integrals. In a recent work[4] I showed that on a general (pseudo-Riemannian) manifold of dimension m, the (vector) space of Killing tensors of rank n has dimension less than or equal to

$$\frac{(m+n-1)!(m+n)!}{(m-1)!m!n!(n+1)!}$$

and following Kalnins and Miller[5] that equality is attained if and only if M is of constant curvature. Moreover, I adduced evidence that on flat spaces the Killing tensors are generated by just the Killing vectors.

Killing tensors appear to have originated in the context of general relativity but naturally they are much more difficult to deal with on a manifold which is not flat. Also, Woodhouse[6] introduced the concepts of Killing pairs and conformal Killing tensors which correspond to integrals of motion which are rational in the momenta and integrals of motion for the null geodesics in relativistic mechanics, respectively.

Returning to (3.1) it is clear that linear integrals of motion are determined by Killing vector fields which preserve V. This is well known from Noether's theorem and so I shall not discuss linear integrals here. Quadratic integrals, which from the preceding comments may be taken in the form $A_{ij} p_i p_j + A$, correspond to rank 2 Killing tensors which also satisfy the conditions.

$$A_{,i} = 2V_{,j} A_{ij}. \tag{3.2}$$

Here A may be eliminated from these conditions leaving several *linear* second-order partial differential equations to be satisfied by V. For the case of two degrees of freedom, conditions (3.2) reduce to a single independent condition which has been the subject of several investigations[1,7-9] and shall not be repeated here. More generally, when using (3.1) to detect polynomial integrals of odd or even degree the second highest degree term is always subject to some linear equations which also involve the components of the Killing tensors. However, for degree 3 constants or higher there will also enter *nonlinear* equations which make the problem of finding such integrals much more complicated. Example (6) in Sec. V gives an example of such a complication.

IV. A SPECIFIC EXAMPLE

I shall next give a rather detailed example of how Eqs. (3.1) may actually be used in practice. Referring to Sec III, I suppose that $m = 2$ and write $x = x_1$, $y = x_2$, $p_x = p_1$, $p_y = p_2$. I also assume that $V = V(x-y)$ and so the quantity $M = \frac{1}{2}(p_x + p_y)$is a constant of motion by Noether's theorem. Besides M and the Hamiltonian H there must be one more functionally independent integral depending on (x, y, p_x, p_y) and one may ask whether this third integral is polynomial in momenta. It is quite straightforward to show that if the polynomial has degree 2 or 3, then up to various inessential additive and multiplicative constants

$$V = x - y \quad \text{or} \quad V = 1/(x-y)^2. \tag{4.1}$$

Now suppose that f is a degree 4 integral. By considering the sequence $f, \{f,M\}, \{\{f,M\},M\}, \ldots$, it is clear that it is sufficient to look for an f whose Killing components are of degree less than or equal to 1. Note that $\{f,M\} \neq 0$, otherwise there would be three mutually commuting integrals $\{H,M,f\}$ which would force f to be dependent on H and M. More generally, one may refer to a polynomial integral as trivial if it can be obtained from polynomial combinations of constants of lower degree. In two dimensions it is certainly true that the Killing tensors are generated by the Killing vectors[4] and so it is sufficient to take the degree 4 term of the integral as

$$\begin{aligned} &A_{ijkl} p_i p_j p_k p_l \\ &\quad = 4(yp_x - xp_y) \\ &\qquad \times (D_1 p_x^3 - 3D_3 p_x^2 p_y + 3D_4 p_x p_y^2 - D_2 p_y^3) \\ &\qquad + E_1 p_x^4 + 4E_3 p_x^3 p_y + 6E_5 p_x^2 p_y^2 \\ &\qquad + 4E_4 p_x p_y^3 + E_2 p_y^4, \end{aligned} \tag{4.2}$$

where the D's and E's are constants.

Now applying conditions (3.1) one obtains the following system of equations where a prime denotes differentiation with respect to the variable $x - y$:

$$\begin{aligned} &A_{11,1} = 4V'(A_{1111} - A_{1112}), \\ &A_{11,2} + 2A_{12,1} = 12V'(A_{1112} - A_{1122}), \\ &A_{22,1} + 2A_{12,2} = 12V'(A_{1122} - A_{1222}), \\ &A_{22,2} = 4V'(A_{1222} - A_{2222}), \end{aligned} \tag{4.3}$$

and

$$\begin{aligned} &A_{,1} = 2V'(A_{11} - A_{12}), \\ &A_{,2} = 2V'(A_{12} - A_{22}). \end{aligned} \tag{4.4}$$

Equations (4.3) yield partial integrability conditions on the A_{ij}: one can use the first pair and last pair to obtain, after differentiation, expressions for $A_{12,11}$ and $A_{12,22}$. Then demand that $A_{12,1122} = A_{12,2211}$. One obtains

$$\begin{aligned} &15(D_1 + D_2 - D_3 - D_4)V''' + (2D_1(x-2y) + 2D_2(2x-y) \\ &\quad + 6D_3 y - 6D_4 x - E_1 + E_2 - 2E_3 + 2E_4)V'''' = 0. \end{aligned} \tag{4.5}$$

It follows since $V = V(x-y)$ that

$$\begin{aligned} &15(D_1 + D_2 - D_3 - D_4)V''' + (3(D_1 + D_2 - D_3 - D_4)(x-y) \\ &\quad - E_1 + E_2 - 2E_3 + 2E_4)V'''' = 0, \end{aligned} \tag{4.6}$$

and

$$(D_1 - D_2 - D_3 + D_4)V''' = 0, \tag{4.7}$$

or else

$$D_1 + D_2 - D_3 - D_4 = D_1 - D_2 - D_3 + D_4 = E_1 - E_2 + 2E_3 - 2E_4 = 0. \tag{4.8}$$

If (4.6) and (4.7) hold, V is of the form

$$V = K(x-y) \quad \text{or} \quad V = Q(x-y) + q/(x-y)^2, \tag{4.9}$$

where K is a cubic polynomial, Q a quadratic polynomial and, q some constant. Next, using (4.4) one obtains the further condition

$$(A_{11} - A_{22})V'' = (A_{11,2} - A_{12,1} - A_{12,2} + A_{22,1})V'. \tag{4.10}$$

It follows from either of conditions (4.9) together with (4.10) that V has one of the forms given by (4.1) and that f is necessarily trivial.

I next turn to the other alternative, i.e., that (4.8) holds. Using the fact that M^4, HM^2, H^2 are all polynomial integrals one may further suppose that either

$$E_1 = E_2 = E_3 = E_4 = E_5, \tag{4.11}$$

or

$$D_1 = -D_2 = 1, \quad E_1 = E_2 = E_3 = E_4 = E_5 = 0. \tag{4.12}$$

Equation (4.11) leads once again to $V = x - y$. Equation (4.12) in conjunction with Eq. (4.10) leads to the following condition where $W' = V$:

$$WW''' + 3(x-y)W'W''' + 3(x-y)W''W'' + 12W'W'' = 0. \tag{4.13}$$

Besides the solutions equivalent to (4.1), (4.13) gives a third possibility, i.e., that $V = 1/(x-y)^{2/3}$. Thus the Hamiltonian given by

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + 1/(x-y)^{2/3}$$

has the quartic integral f given by

$$f = 4(yp_x - xp_y)(p_x - p_y)^3 + \frac{8(p_x - p_y)((yp_x - xp_y) - (x-y)(p_x + p_y))}{(x-y)^{2/3}} + \frac{32(x+y)}{(x-y)^{4/3}}.$$

Moreover, this is essentially the only system which admits a nontrivial quartic polynomial.

The result may be generalized as follows. Define the Hamiltonians H_k, $k = 0,1,2,\ldots$, by

$$H_k = \tfrac{1}{2}(p_x^2 + p_y^2) + 1/(x-y)^{2/(2k+1)}.$$

Then f_k is an integral of degree $2(k+1)$ where

$$\frac{1}{16}f_k = (p_x + p_y)\left(\frac{1}{2^{2k+1}}\binom{k}{0}\frac{2k+1}{2k+1}(x-y)^{(2k+1)/(2k+1)}(p_x - p_y)^{2k+1} + \frac{1}{2^{2k-1}}\binom{k}{1}\frac{2k+1}{2k-1}(x-y)^{(2k-1)/(2k+1)}(p_x - p_y)^{2k-1} + \cdots + \frac{1}{2}\binom{k}{k}\frac{2k+1}{1}(x-y)^{1/(2k+1)}(p_x - p_y)\right) - 2(x+y)\left(\frac{1}{4}(p_x - p_y)^2 + \frac{1}{(x-y)^{2/(2k+1)}}\right)^{k+1}.$$

V. OTHER EXAMPLES

(1) Consider the system with m degrees of freedom whose Hamiltonian is given by

$$H = \tfrac{1}{2}p_i p_i + e,$$

where e is a homogeneous function of degree -2 and also $\{\Sigma_{j=1}^m p_j, e\} = 0$. This system is a variation of the Calogero system.[10-12] The following integrals were found using (3.1):

$$E = x_i x_i p_j p_j - x_i x_j p_i p_j + 2x_i x_i e,$$

$$F = \left(\sum_{i=1}^m x_i\right)p_j p_j - x_j p_j \left(\sum_{i=1}^m p_i\right) + 2\left(\sum_{i=1}^m x_i\right)e.$$

(2) As another variation on the Calogero system consider the system with m degrees of freedom whose Hamiltonian is given by

$$H = \tfrac{1}{2}p_i p_i + e + f(x_i x_i),$$

where e is a homogeneous function of degree -2, $\{\Sigma_{j=1}^m p_j, e\} = 0$, and f is any function of $x^2 = \mathbf{x}\cdot\mathbf{x}$. This time one has the integrals

$$E = x_i x_i p_j p_j - x_i x_j p_i p_j + 2x_i x_i e,$$

$$D = \left(\sum_i (x_i)p_j - x_j \sum_i (p_i)\right)\left(\sum_i (x_i)p_j - x_j \sum_i (p_i)\right) + 2\left(\sum_i x_i\right)^2 (e+f),$$

so that for $m = 3$ this system is completely integrable.

(3) In this example I consider a system with two degrees of freedom whose Hamiltonian is given by

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + V(x^2 + y^2).$$

This is the angular momentum analog of the example treated in Sec. IV so that $yp_x - xp_y$ is an integral. If one asks for those V which have nontrivial quadratic or cubic integrals it turns out that in the former case

$$V = x^2 + y^2 \quad \text{or} \quad V = 1/(x^2 + y^2)^{1/2}.$$

In the latter case one finds there are no V's which have nontrivial cubic integrals. This underlines the importance of the harmonic oscillator and Kepler potentials which is indeed what these two are.

(4) The system with two degrees of freedom whose Hamiltonian is given by

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + x^2 y - y^3/3$$

was considered. This is the infamous Henon–Heiles system of celestial mechanics. Using (3.1) it was found that the system has no integrals of degree 1, 2, 3, or 4 besides H itself. This provides fragmentary evidence to corroborate the conclusion of Leach.[13]

(5) In the next example I consider a class of systems which includes the type considered in special relativity. Let H be the Hamiltonian where g_{ij} is a flat metric of any signature and

$$H = (1 + g^{ij}p_i p_j)^{1/2} + V.$$

The analog of (3.1) gives, where ";" denote the covariant derivative with respect to g_{ij},

$$A^{a_1\cdots a_{n-1}}V_{;i} = 0,$$
$$A^{a_1\cdots a_{n-2}}V_{;i} = 0,$$
$$\vdots$$
$$A^{a_1 i}V_{;i} = 0,$$
$$A^{i}V_{;i} = 0.$$

It follows that in looking for polynomial integrals it is sufficient to consider just homogeneous polynomials. Also, this system has precisely the same *linear* integrals as the classical Hamiltonian H' given by

$$H' = \tfrac{1}{2}g^{ij}p_i p_j + V.$$

(6) In this last example I will first of all consider the problem of trying to obtain cubic integrals for systems in general, then specialize to a particular kind of system with two degrees of freedom. The cubic integral may be assumed to have the form

$$A_{ijk}\,p_i\,p_j\,p_k + A_i\,p_i, \tag{5.1}$$

where A_{ijk} is a Killing tensor. One of the two remaining conditions from (3.1) is

$$A_{(i,j)} = 3V_{,k}A_{ijk}. \tag{5.2}$$

Now differentiate (5.2) twice to obtain

$$A_{(i,j)lm} = 3V_{,klm}A_{ijk} + 3V_{,kl}A_{ijk,m} + 3V_{,km}A_{ijk,l} + 3V_{,k}A_{ijk,lm}. \tag{5.3}$$

The left-hand side of (5.3) is symmetric in all four indices and so insisting that the right-hand side be symmetric too, gives the following system of linear, third order, partial differential equations for V:

$$A_{ijk}V_{,klm} + A_{ijk,m}V_{,kl} + A_{ijk,l}V_{,km} + A_{ijk,lm}V_{,k} = A_{jlk}V_{,kim} + A_{ljk,m}V_{,ki} + A_{ljk,i}V_{,km} + A_{ljk,im}V_{,k}. \tag{5.4}$$

Clearly one also obtains analogous linear conditions on V starting with any polynomial constant whose degree is bigger than 1.

Now I specialize to the case $m = 2$ and consider, on grounds of tractability, a cubic integral of the form

$$(yp_x - xp_y)^3 + Ap_x + Bp_y,$$

where again I write $x = x_1$, $y = x$, $p_x = p_1$, $p_y = p_2$, and $A = A_1$, $B = A_2$. The remaining conditions of (3.1) may be written as

$$\frac{\partial A}{\partial x} = 3y^2\left(y\frac{\partial V}{\partial x} - x\frac{\partial V}{\partial y}\right),$$
$$\frac{\partial A}{\partial y} + \frac{\partial B}{\partial x} = -6xy\left(y\frac{\partial V}{\partial x} - x\frac{\partial V}{\partial y}\right), \tag{5.5}$$
$$\frac{\partial B}{\partial y} = 3x^2\left(y\frac{\partial V}{\partial x} - x\frac{\partial V}{\partial y}\right),$$

and

$$A\frac{\partial V}{\partial x} + B\frac{\partial V}{\partial y} = 0. \tag{5.6}$$

Condition (5.4) is most easily obtained from (5.5) directly, much as (4.5) was obtained in Sec. IV. There is a single equation which is

$$x^2yV_{xxx} - (x^3 - 2xy^2)V_{xxy} + (y^3 - 2x^2y)V_{xyy} - xy^2V_{yyy} + 8xyV_{xx} + 8(y^2 - x^2)V_{xy} - 8xyV_{yy} + 12yV_x - 12xV_y = 0. \tag{5.7}$$

The solution of (5.7) is

$$V = f(x^2 + y^2) + g + h, \tag{5.8}$$

where f is an arbitrary function and g and h are homogeneous functions of degree -2 and -3 respectively. Thus, imposing the second condition in (3.1) imposes strong conditions on the form of V.

In view of (5.8) it is convenient to change coordinates so that

$$\zeta = x^2 + y^2, \quad \eta = y/x.$$

In order that the transformation be canonical one must also have that

$$p_x = 2xp_\zeta - (y/x^2)p_\eta, \quad p_y = 2yp_\zeta + (1/x)p_\eta$$

and the Hamiltonian, in view of (5.8) may be written as

$$H = 2\zeta p_\zeta^2 + f(\zeta) + \frac{(1+\eta^2)p_\eta^2 + G(\eta)}{2\zeta} + \frac{H(\eta)}{\zeta^{3/2}}, \tag{5.9}$$

for some functions G and H. The cubic integral now assumes the form

$$(1+\eta^2)^3p_\eta^3 + ap_\zeta + bp_\eta, \tag{5.10}$$

for some functions a and b. It remains to satisfy the last condition in (3.1) as well as to relate a and b to f, G and H. One finds that

$$2\zeta\frac{\partial a}{\partial \zeta} = a, \tag{5.11}$$

$$4\zeta^2\frac{\partial b}{\partial \zeta} + (1+\eta^2)^2\frac{\partial a}{\partial \eta} = 0, \tag{5.12}$$

$$\frac{a(1+\eta^2)}{2\zeta^2} + \frac{(1+\eta^2)}{\zeta}\frac{\partial b}{\partial \eta} - \frac{2b\eta}{\zeta} = 3(1+\eta^2)^2\left(\frac{G'(\eta)}{\zeta} + \frac{H'(\eta)}{\zeta^{3/2}}\right), \tag{5.13}$$

but the last condition (5.6) has still not been applied. Still without applying it, it follows that the cubic integral has the form

$$(1+\eta^2)^3p_\eta^3 + \theta(\eta)\zeta^{1/2}p_\zeta + \left(\frac{(1+\eta^2)^2\theta'(\eta)}{2\zeta^{1/2}} + 3(1+\eta^2)G(\eta)\right)p_\eta, \tag{5.14}$$

where θ is a function of η satisfying

$$\theta + (1+\eta^2)^2\theta'' = 6(1+\eta^2)H'. \tag{5.15}$$

When (5.6) is applied one finds that the function f is a sum of three functions homogeneous of degrees -1, -2, -3, respectively. Then one may argue in several stages that there is no loss of generality in supposing that $f \equiv 0$ and $G \equiv 0$. The cubic integral then has the form

$$(1+\eta^2)^2 p_\eta^3 + \theta\zeta^{1/2} p_s + ((1+\eta^2)^2\theta'/2\zeta^{1/2})p_\eta,$$

where in addition to (5.15), θ and H are also bound by the relation

$$3\theta H = (1+\eta^2)^2\theta' H'. \tag{5.16}$$

Next, setting

$$K \sec z = \theta \text{ and } \eta = \tan z \tag{5.17}$$

(5.15) and (5.16) are transformed, respectively, to

$$K'' + 2K = 6H' \cos z, \tag{5.18}$$

$$3HK = H'K' + H'K \tan z, \tag{5.19}$$

where a prime denotes differentiation with respect to z. One can obtain a single, albeit rather complex, third-order equation for K by differentiating each of (5.18) and (5.19) with respect to z and then using all four equations to eliminate H, H', and H''.

Finally, I shall summarize the results of this example using the original notation. It has been shown that the only systems which have a potential of the type given by (5.8) which have an integral of the form $(yp_x - xp_y)^3 + Ap_x + Bp_y$ are those which have a Hamiltonian given by

$$\tfrac{1}{2}(p_x^2 + p_y^2) + H(y/x)/(x^2+y^2)^{3/2}.$$

In this case the integral is given by

$$-(yp_x - xp_y)^3 + \frac{1}{2(x^2+y^2)^{1/2}}\left[Kx(xp_x + yp_y) - \left(K\frac{\sqrt{x^2+y^2}}{x}\right)'(yp_x - xp_y)\right],$$

where a prime denotes differentiation with respect to $z = \arctan(y/x)$. Moreover, H and K are related by (5.18) and (5.19)—conditions which imply that H depends on three arbitrary constants.

ACKNOWLEDGMENTS

The author would like to thank the referee for several useful suggestions; he is also grateful to Marek Kossowski, William Shadwick, Felix Pirani, Robert Gardner, and, above all, Michael Crampin for illuminating discussions.

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A viewpoint of Kaluza–Klein type in elasticity theory

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(Received 2 August 1983; accepted for publication 22 June 1984)

An N-dimensional anisotropic elastic body without the interior gravity is, under some conditions concerning the N th dimension, equivalent to an $(N-1)$-dimensional isotropic elastic body under the influence of the interior gravity. According to this theorem, our method of solving the equation of free motion of anisotropic elastic bodies includes Bromwich's method of solving the equation of motion of incompressible isotropic elastic bodies under the influence of the interior gravity.

PACS numbers: 03.40.Dz, 04.20.Me

I. INTRODUCTION

Long ago Lamb[1] invented an ingenious method of solving the equation of free motion of isotropic elastic bodies. Lamb's method reduces the equation of elastic motion to some Helmholtz equations. Bromwich[2] generalized Lamb's method to the equation of motion of incompressible isotropic elastic bodies under the influence of the interior gravity. Bromwich's method also reduces the equation of elastic motion to some Helmholtz equations. Bromwich showed, by using his method, that the period of the spheroidal vibrations of a sphere of the same mass and size as the Earth and as rigid as steel would be diminished from 66 to 55 min by the natural gravitation of the parts of the sphere.[3] On the other hand, we generalized, in a recent papaer,[4] Lamb's method to the equation of free motion of C_∞ anisotropic elastic bodies.[5] The C_∞ generalization also reduces the equation of elastic motion to some Helmholtz equations. Using the C_∞ generalization, we have obtained all the exact solutions of the guided elastic waves of C_∞ anisotropic elastic cylinders.[6] Thus, Lamb's method was generalized to two physical systems which are quite different from each other.

We shall prove that the C_∞ generalization includes Bromwich's method as a special case. The two generalizations correspond to two quite different physical systems, so it seems to be strange that one includes another as a special case. However, a viewpoint of Kaluza–Klein type will make this strangeness melt away. In the approach of Kaluza–Klein type, an object in a higher-dimensional space-time or space having some symmetries describes different physical objects in a lower-dimensional space-time or space. For example, in Kaluza–Klein's unified field theory,[7] a metric field in a five-dimensional space-time describes a metric field and an electromagnetic field in a four-dimensional space-time. In general relativity, if a four-dimensional space-time is vacuum, stationary, and axial symmetric, the space-time is known to be equivalent to a two-dimensional space with matter fields.[8] We shall see that elasticity theory also has such a structure as these examples.

We treat a C_∞ elastic body in an N-dimensional Euclidean space, but we neglect the interior gravity. Latin indices are used to label an arbitrary Cartesian coordinate system in the N-dimensional Euclidian space. We write ρ for the mass density, n^i for the unit vector along the C_∞ direction at each point, c_{ijkl} for the stiffness tensor, u^i for the displacement vector, $s_{ij}(\equiv u_{(i,j)})$ for the strain tensor, and T^{ij} for the stress tensor. Then the free motion of the N-dimensional C_∞ elastic body is given by the equation of elastic motion

$$\rho\frac{\partial^2 u^i}{\partial t^2} = T^{ij}{}_{,j} \tag{1.1}$$

with a constitutive equation, called Hooke's law,

$$T^{ij} = c^{ijkl}s_{kl}. \tag{1.2}$$

First we shall prove that the C_∞ elastic body has such a structure as theories of Kaluza–Klein type: The N-dimensional C_∞ elastic body without the interior gravity is equivalent to an $(N-1)$-dimensional isotropic elastic body under the influence of the interior gravity under the following conditions concerning the N th dimension.

(C1) The n^i is a parallel vector field: $n^i{}_{,j} = 0$. So, selecting a specifical Cartesian coordinate system, we can make the direction of the N th coordinate axis coincide with the n^i direction. We use such a specific Cartesian coordinate system $(x^1,...,x^N)$. We also use Greek indices to label a specific $(N-1)$-dimensional Cartesian coordinate system $(x^1,...,x^{N-1})$, which covers an $(N-1)$-dimensional Euclidean space whose normal vector is the n^i.

(C2) The displacement vector u^i is sinusoidal along the n^i, and it has the period $2\pi/k$: $u^i{}_{,k}n^k = iku^i$. And also the k is infinitesimal: $k\to 0$.

(C3) The nonvanishing stiffness components concerning the n^i direction are infinitely stiff: $c_{NNNN}\to\infty$, $c_{\mu\mu NN}\to\infty$, $c_{N\mu N\mu}\to\infty$.

The limit values 0 and ∞ in conditions (C2) and (C3) will make Eq. (1.1) vague. To avoid the vagueness, we shall have to specify sequences of numbers leading to the limit values. In the following proof, such sequences of numbers will be specified.

Successively, using the above theorem, we shall prove the statement described in the beginning: The C_∞ generalization includes Bromwich's method as a special case.

II. THE PROOF OF THE THEOREM

The stiffness tensor c_{ijkl} with the C_∞ symmetry is invariant under the rotation around the n^i. Therefore, the tensor must be constructed only from scalars n^i and the $(N-1)$-dimensional metric tensor and alternating tensor in the quotient space modulo n^i. The most general expression of the tensor is then as follows:

$$\begin{aligned} c_{ijkl} = {} & \lambda h_{ij}h_{kl} + 2\mu h_{i(k}h_{l)j} + \xi(h_{ij}n_kn_l + h_{kl}n_in_j) \\ & + 4\eta n_{(i}h_{j)(k}n_{l)} + \zeta n_in_jn_kn_l, \end{aligned} \tag{2.1}$$

where $\lambda, \mu, \xi, \eta, \zeta$ are scalars. They are assumed to be constant. The h_{ij} is the $(N-1)$-dimensional metric tensor, and it

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is $h_{ij}=0$ for $i\neq j$, $h_{\mu\mu}=1$, $h_{NN}=0$ in the specifical Cartesian coordinate system.

Substituting Eqs. (1.2) and (2.1) into Eq. (1.1), and projecting the resulting equation into the $(N-1)$-dimensional space and into the n^i direction, we have

$$\rho\frac{\partial^2 u^\mu}{\partial t^2}=\mu\Delta_\perp u^\mu+(\mu+\lambda)\delta_{,}{}^{\mu}-\eta k^2 u^\mu+(\xi+\eta)s_{,}{}^{\mu}, \tag{2.2}$$

$$\rho\frac{\partial^2 w}{\partial t^2}=\eta\Delta_\perp w+ik\zeta s+ik(\xi+\eta)\delta, \tag{2.3}$$

where we have used conditions (C1) and (C2). The $\Delta_\perp\equiv\partial_\mu\,\partial^\mu$ is the Laplacian in the $(N-1)$-dimensional Euclidean space, and $w\equiv u^N$, $\delta\equiv u^\mu{}_{,\mu}$, $s\equiv w_{,i}n^i$ are the displacement along the n^i, the $(N\text{-}1)$-dimensional volumetric strain, the strain along the n^i, respectively. Differentiation of Eq. (2.3) along the n^i gives

$$\rho\frac{\partial^2 s}{\partial t^2}=\eta\Delta_\perp s-k^2\zeta s-k^2(\xi+\eta)\delta, \tag{2.4}$$

where we have used condition (C2).

Let us normalize the six N-dimensional matter constants $\rho,\lambda,\mu,\xi,\eta,\zeta$ by introducing an arbitrary constant L with the dimension of length: $\tilde\rho\equiv L\rho$, $\tilde\lambda\equiv L\lambda$, and so on. The $\tilde\rho$ has then the dimension of $(N-1)$-dimensional mass densities, and the $\tilde\lambda$, $\tilde\mu$, $\tilde\xi$, $\tilde\eta$, $\tilde\zeta$ have the dimension of $(N-1)$-dimensional elastic constants. Instead of four constants $\tilde\xi$, $\tilde\eta$, $\tilde\zeta$, k, we define four new constants:

$$M^2\equiv\frac{\tilde\eta k^2}{(\tilde\lambda+2\tilde\mu)},\quad m^2\equiv\frac{\tilde\zeta k^2}{\tilde\eta},$$
$$v^2\equiv\frac{\tilde\eta}{\tilde\rho},\quad 4\pi G\equiv\frac{(\tilde\xi+\tilde\eta)^2k^2}{\tilde\rho^2\tilde\eta}. \tag{2.5}$$

Moreover, let us normalize the variable s as follows:

$$\phi\equiv-[(\tilde\xi+\tilde\eta)/\tilde\rho]s. \tag{2.6}$$

Using $\phi,\tilde\rho,\tilde\lambda,\tilde\mu$ instead of s,ρ,λ,μ, and M^2,m^2,v^2,G instead of ξ,η,ζ,k, we see that Eqs. (2.2) and (2.4) turn out to be[9]

$$\tilde\rho\frac{\partial^2 u^\mu}{\partial t^2}=\tilde\mu\Delta_\perp u^\mu+(\tilde\mu+\tilde\lambda)\delta_{,}{}^{\mu}-(\tilde\lambda+2\tilde\mu)M^2u^\mu-\phi_{,}{}^{\mu}, \tag{2.7}$$

$$\left(\Delta_\perp-\frac{1}{v^2}\frac{\partial^2}{\partial t^2}-m^2\right)\phi=-4\pi G\tilde\rho\delta. \tag{2.8}$$

Now we consider the limit values described in conditions (C2) and (C3). As is seen from Eq. (2.1), the limit values of condition (C3) are equivalent to $\xi\to\infty$, $\eta\to\infty$, $\zeta\to\infty$. Accordingly, the v^2 is infinite, but the limit values of M^2, m^2, G are indefinite. Their limit values are dependent on sequences of numbers leading to $k\to0$, $\xi\to\infty$, $\eta\to\infty$, $\zeta\to\infty$. There are sequences of numbers which give

$$v^2\to\infty,\quad M^2\to0,\quad m^2\to0,\quad M^2/m^2\to\text{a finite value},$$
$$G\to\text{a finite value}, \tag{2.9}$$

because we can solve Eq. (2.5) as

$$k^2=\frac{(\tilde\lambda+2\tilde\mu)M^2}{\tilde\rho v^2},\quad \tilde\xi=\tilde\rho v^2\left(\left(\frac{4\pi G\tilde\rho^2}{(\tilde\lambda+2\tilde\mu)M^2}\right)^{1/2}-1\right),$$
$$\tilde\eta=\tilde\rho v^2,\quad \tilde\zeta=(\tilde\rho v^2)^2\frac{m^2}{(\tilde\lambda+2\tilde\mu)M^2}, \tag{2.10}$$

and so the limit values (2.9) give $k\to0$, $\xi\to\infty$, $\eta\to\infty$, $\zeta\to\infty$.[10] The specifical limit values (2.9) reduce Eqs. (2.7) and (2.8) to

$$\tilde\rho\frac{\partial^2 u^\mu}{\partial t^2}=\tilde\mu\Delta_\perp u^\mu+(\tilde\mu+\tilde\lambda)\delta_{,}{}^{\mu}-\tilde\rho\phi_{,}{}^{\mu}, \tag{2.11}$$

$$\Delta_\perp\phi=-4\pi G\tilde\rho\delta. \tag{2.12}$$

The reduced equations (2.11) and (2.12) allow us an interesting physical interpretation. We consider a $(N-1)$-dimensional isotropic elastic body under the influence of the interior gravity. Let us decompose the displacement vector into the displacement of the static equilibrium state and the dynamical deviation from the static state. In the same way, we decompose the potential of the interior gravity into two parts. Then, as is easily ascertained, the dynamical deviations of the displacement vector and the interior gravitational potential satisfy Eqs. (2.11) and (2.12).[11] The u^μ and ϕ are then the dynamical displacement vector and the dynamical interior gravitational potential, respectively. The $G,\tilde\rho,\tilde\lambda$, and $\tilde\mu$ are Newton's gravitational constant, the mass density, and Lamè's elastic constants, respectively.

If the argument above is conversely followed, we can easily see that the two equations (2.11) and (2.12) in the $(N-1)$-dimensional Euclidean space can be combined into only one equation (1.1) in the N-dimensional Euclidean space under conditions (C1)–(C3).

In the above proof, we have decomposed the displacement and the interior gravitational potential into the static equibrium parts and the dynamical deviation parts. If you wish, it is possible to avoid the decomposition. To see it, let us shift the u^μ by the position vector x^μ normalized with the dimension $(N\text{-}1)$: $\tilde u^\mu\equiv[1/(N-1)]x^\mu-u^\mu$. Moreover, let us transform the ϕ as $\tilde\phi\equiv-\phi$. Using the $\tilde u^\mu$ and $\tilde\phi$ instead of u^μ and ϕ, we can rewrite Eqs. (2.11) and (2.12) as

$$\tilde\rho\frac{\partial^2\tilde u^\mu}{\partial t^2}=\tilde\mu\Delta_\perp\tilde u^\mu+(\tilde\mu+\tilde\lambda)\tilde\delta_{,}{}^{\mu}-\tilde\rho\tilde\phi_{,}{}^{\mu}, \tag{2.13}$$

$$\Delta_\perp\tilde\phi=4\pi G\tilde\rho(1-\tilde\delta), \tag{2.14}$$

where $\tilde\delta\equiv\tilde u^\mu{}_{,\mu}=1-\delta$. If the transformed $\tilde u^\mu$ and $\tilde\phi$ are reinterpreted as the displacement vector and the interior gravitational potential, Eqs. (2.13) and (2.14) are exactly the equation of motion and Newton's law of gravity for the $(N-1)$-dimensional isotropic elastic body under the influence of the interior gravity.

III. BROMWICH'S METHOD AS A SPECIAL CASE

Recently we exploited a method of solving Eqs. (2.2) and (2.3) for the vibrations with an angular frequency ω. The method is a generalization of Lamb's method for isotropic bodies to C_∞ bodies. According to the C_∞ generalization,[12] the s consists of two terms

$$s=s(p)+s(q). \tag{3.1}$$

Each term is determined by Helmholtz equations

$$(\Delta_\perp+p^2)s(p)=0,\quad (\Delta_\perp+q^2)s(q)=0, \tag{3.2}$$

where

$$\frac{p^2+q^2}{2}\equiv\frac{(\lambda+2\mu+\eta)\rho\omega^2-[\zeta(\lambda+2\mu)-\xi(\xi+2\eta)]k^2}{2\eta(\lambda+2\mu)},$$

$$\frac{p^2-q^2}{2}\equiv\left\{\left(\frac{(\lambda+2\mu+\eta)\rho\omega^2-[\zeta(\lambda+2\mu)-\xi(\xi+2\eta)]k^2}{2\eta(\lambda+2\mu)}\right)^2-\frac{(\rho\omega^2)^2-\rho\omega^2(\eta+\zeta)k^2+\eta\zeta k^4}{\eta(\lambda+2\mu)}\right\}^{1/2}. \tag{3.3}$$

The δ also consists of two terms

$$\delta=\delta(p)+\delta(q). \tag{3.4}$$

Each term is given by

$$\delta(\gamma)=[(-\eta\gamma^2+\rho\omega^2-\zeta k^2)/(\xi+\eta)k^2]s(\gamma),$$
$$\gamma=p,q. \tag{3.5}$$

The displacements u^μ and w are constructed in the following way:

$$u^\mu=u_{(1)}{}^\mu+u_{(2)}{}^\mu, \tag{3.6}$$
$$w=s/ik. \tag{3.7}$$

The $u_{(1)}{}^\mu$ is given by

$$u_{(1)}{}^\mu=-p^{-2}\delta(p)_{,}{}^\mu-q^{-2}\delta(q)_{,}{}^\mu. \tag{3.8}$$

The $u_{(2)}{}^\mu$ is determined by a vector Helmholtz equation with a constraint equation:

$$(\Delta_\perp+\kappa^2)u_{(2)}{}^\mu=0,\quad u_{(2)}{}^\mu{}_{,\mu}=0, \tag{3.9}$$

where

$$\kappa^2\equiv(\rho\omega^2-\eta k^2)/\mu. \tag{3.10}$$

Thus, the C_∞ generalization reduces the equations of motion (2.2) and (2.3) into Helmholtz equations (3.2) and (3.9).

Let us now consider the limit values (2.9). The p^2, q^2, and κ^2 then reduce to

$$p^2=(\tilde\rho\omega^2+4\pi G\tilde\rho^2)/(\tilde\lambda+2\tilde\mu), \tag{3.11a}$$
$$q^2=0, \tag{3.11b}$$
$$\kappa^2=\tilde\rho\omega^2/\tilde\mu. \tag{3.11c}$$

Rewriting Eqs. (3.1) and (3.2) by using Eqs. (3.11) and (2.6), we have

$$\phi=\phi(p)+\phi(q), \tag{3.12}$$

and

$$(\Delta_\perp+p^2)\phi(p)=0, \tag{3.13a}$$
$$(\Delta_\perp+q^2)\phi(q)=0. \tag{3.13b}$$

Equations (3.12) and (3.13) show that the potential ϕ is determined by two Helmholtz equations. Equations (3.5) turn out to be relations between $\phi(\gamma)$ and $\delta(\gamma)$:

$$p^{-2}\delta(p)=(1/4\pi G\tilde\rho)\phi(p), \tag{3.14a}$$
$$q^{-2}\delta(q)=-\omega^{-2}\phi(q). \tag{3.14b}$$

Owing to Eq. (3.11b), Eq. (3.14b) yields

$$\delta(q)=0. \tag{3.15}$$

Accordingly, Eq. (3.14a) turns out to be

$$p^{-2}\delta=(1/4\pi G\tilde\rho)\phi(p). \tag{3.16}$$

Owing to Eqs. (3.15) and (3.14b), Eq. (3.8) turns out to be

$$u_{(1)}{}^\mu=-p^{-2}\delta_{,}{}^\mu+\omega^{-2}\phi(q)_{,}{}^\mu. \tag{3.17}$$

Equations (3.11)–(3.13), (3.16), (3.17), (3.9), and (3.6) form a method of solving Eqs. (2.11) and (2.12). The potential ϕ is determined by adding two potentials $\phi(p)$ and ϕ(q) which are the solutions of the Helmholtz equations (3.13). The $\phi(p)$ yields the $(N-1)$-dimensional volumetric strain δ through Eq. (3.16). The displacement vector u^μ is obtained by adding the $u_{(1)}{}^\mu$ that are calculated from δ and $\phi(q)$ according to Eq. (3.17) and the $u_{(2)}{}^\mu$ that is the solution of the vector Helmholtz equation (3.9) with the constraint equation. Thus the equation of motion (2.11) and Newton's law of gravity (2.12) have been reduced to Helmholtz equations.

Successively, we consider the incompressible limit

$$p_1\equiv\lim_{\substack{\tilde\lambda\to\infty\\ \delta\to0}}\tilde\lambda\delta. \tag{3.18}$$

In this limit, the equation of motion (2.11) and Newton's law of gravity (2.12) turn out to be

$$\tilde\rho\frac{\partial^2u^\mu}{\partial t^2}=\tilde\mu\Delta_\perp u^\mu+p_{1,}{}^\mu-\tilde\rho\phi_{,}{}^\mu, \tag{3.19}$$
$$\Delta_\perp\phi=0. \tag{3.20}$$

The incompressible limit for Eqs. (3.11)–(3.13), (3.16), (3.17), (3.9), and (3.6), which form a method of solving Eqs. (2.11) and (2.12), must produce a method of solving Eqs. (3.19) and (3.20). The limit $\tilde\lambda\to\infty$ gives $p^2\to0$. Thus, owing to Eqs. (3.16), (3.11a), and (3.18), Eq. (3.13a) turns out to be

$$\Delta_\perp p_1=0. \tag{3.21}$$

Then, in order that Eq. (3.13b) is consistent with Eq. (3.20), we must have

$$\phi(p)=0. \tag{3.22}$$

On the other hand, Eq. (3.16) yields

$$\lim_{\substack{\tilde\lambda\to\infty\\ \delta\to0}}p^{-2}\delta=\frac{p_1}{\tilde\rho\omega^2+4\pi G\tilde\rho^2}=\frac{\phi(p)}{4\pi G\tilde\rho}. \tag{3.23}$$

In order that Eq. (3.23) is consistent with Eq. (3.22), we must have

$$G=0. \tag{3.24}$$

It seems that Eq. (3.24) contradicts the interpretation that the G is Newton's gravitational constant. However this is not so, because in the incompressible limit both the equation of motion (3.19) and Newton's law of gravity (3.20) do not include G. On account of Eqs. (3.23), (3.24), (3.22), and (3.11c), Eq. (3.17) turns out to be

$$u_{(1)}{}^\mu=-(\tilde\rho\omega^2)^{-1}p_{1,}{}^\mu+\omega^{-2}\phi_{,}{}^\mu$$
$$=-(\tilde\mu\kappa^2)^{-1}(p_1-\tilde\rho\phi)_{,}{}^\mu\equiv-(\tilde\mu\kappa^2)^{-1}\varphi_{,}{}^\mu. \tag{3.25}$$

Equations (3.20) and (3.21) yield the equation for the φ:

$$\Delta_\perp\varphi=0. \tag{3.26}$$

Equations (3.26), (3.25), (3.11c), (3.9), and (3.6) form a method of solving Eqs. (3.19) and (3.20). Thus, the equation of motion (3.19) and Newton's law of gravity (3.20) have been reduced to Helmholtz equations. This method is nothing else but Bromwich's method of solving incompressible isotropic elastic bodies under the influence of the interior gravity.[13] Accordingly, the C_∞ generalization includes Bromwich's method as a special case.

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[4]T. Obata and J. Chiba (to be published). Most of this work has been already announced at a symposium held by the Research Committee of Electro-Magnetic Theory under the auspices of the I. E. E. of Japan, October 1983. A limited number of manuscripts (Manuscript No. EMT-83-51) was distributed by the Research Committee.

[5]In the case that each specifical axis of minute monocrystals constituting a polycrystal is arrayed along a specifical direction of the polycrystal and other axes are random, the polycrystal is called to be cylindrically symmetric. The symmetry is expressed by the symbol C_∞. The C_∞ is equivalent to the C_6 in respect to elastic properties. The C_6 is a point group. For details, see any standard textbook concerning crystals.

[6]T. Obata and J. Chiba (to be published). Most of this work has been already announced at a symposium held by the Research Committee of Electro-Magnetic Theory under the auspices of the I.E.E. of Japan, October 1983. A limited number of manuscripts (Manus. No. EMT-83-52) was distributed by the Research Committee.

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[9]According to Eq. (2.8), v is the propagation velocity of ϕ, m is a masslike quantity, and G is a coupling constant. Here M is also a masslike quantity, because differentiation of Eq. (2.7) with respect to x^μ yields

$$\left(\Delta_\perp - \frac{\tilde{\rho}}{\tilde{\lambda}+2\tilde{\mu}}\frac{\partial^2}{\partial t^2} - M^2\right)\delta = \frac{\tilde{\rho}}{\tilde{\lambda}+2\tilde{\mu}}\Delta_\perp\phi.$$

[10]Any sequences of numbers leading to the order of infinity $k^{-2}\sim\tilde{\eta}^{1+2\alpha}$, $\tilde{\xi}\sim\tilde{\eta}^{1+\alpha}$, $\tilde{\zeta}\sim\tilde{\eta}^2$ with $\alpha>0$ yield the limit values (2.9). For example, $k_n\equiv k_0 2^{-3n/2}$, $\xi_n\equiv\xi_0 2^{2n}$, $\eta_n\equiv\eta_0 2^n$, $\zeta_n\equiv\eta_0 2^{2n}$ $(n=1,2,\ldots)$.

[11]Under the volumetric strain δ, any infinitesimal volume dV changes to $dV(1+\delta)$, so the mass density $\tilde{\rho}$ changes to $\tilde{\rho}/(1+\delta)=\tilde{\rho}(1-\delta)+O(\delta^2)$. Accordingly, $[\tilde{\rho}(1-\delta)]_{\text{static equibrium part}}=\tilde{\rho}(1-\delta_{\text{static equibrium part}})$, $[\tilde{\rho}(1-\delta)]_{\text{dynamical deviation part}}=-\tilde{\rho}\delta_{\text{dynamical deviation part}}$.

[12]The C_∞ generalization in Ref. 4 was done for $n=3$. However, as is easily ascertained, any relations in Ref. 4 hold for arbitrary dimensions.

[13]Our ϕ and φ correspond to Bromwich's $-V$ and ϕ, respectively.

Multifrequency inverse problem for the reduced wave equation: Resolution cell and stability

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(Received 15 February 1984; accepted for publication 1 June 1984)

The multifrequency inverse problem associated with the reduced wave equation $\Delta u + k^2 n^2(x)u = 0, x \in R^3$ is examined for the case where the data set is sparse. The resolution cell or solution set is examined in detail and is shown to be an infinite-dimensional manifold. The concept of stability is introduced. It is shown that the intrinsic condition of structural stability to the inverse process selects out a preferred set of solutions from the solution set. The structural stability of various iterative schemes used in the inverse process are examined.

PACS numbers: 03.40.Kf

I. INTRODUCTION

In a previous paper[1] the multifrequency inverse problem associated with the reduced wave equation

$$\Delta u + k^2 n^2(x)u = 0, \quad x \in R^3 \tag{1}$$

was treated for the sparse data case. All that was specified about $n(x)$ was that it was real, piecewise continuous, and equal to unity outside a given domain D. An iterative technique was developed to solve the inverse system using no other *a priori* knowledge on $n(x)$. Here some of the details in the theory behind the method are examined, and it is shown that the technique employed did contain a natural intrinsic condition that selected a stable solution.

There are two main items that are concentrated on here. Because of the nonuniqueness of the inverse problem with sparse data, the structure of the solution set (resolution cell) is examined in some detail. In particular, it is shown that the solution set is an infinite-dimensional manifold. If however $v(x)$, where

$$v(x) = n^2(x) - 1, \tag{2}$$

is restricted to lie in a given $2N$-dimensional subspace, the solution set will (under general conditions) consist of isolated points. But such solutions will depend critically upon the choice of subspace, and can be quite different for different subspaces. This feature of the solution set being an infinite-dimensional manifold whose intersection with a $2N$-dimensional subspace is an isolated point set, is a serious problem for the sparse data case. This has been recognized by various members of the scientific community, Backus and Gilbert,[2] Bevensee,[3] and Bertero and De Mol,[4] who have developed various regularization techniques for the associated linearized problem. For the nonlinear problem, it is shown here that the additional requirement of structural stability will select out a preferred set of solutions from the solution set.

It should be pointed out that, although the nonuniqueness of the problem under consideration is well-known,[5,6] the more difficult question concerning the structure of the solution set for the full nonlinear problem has not been examined. This knowledge is essential in order to examine the effect of the requirement of structured stability on the solution set, and to show that it is a viable constraint.

II. INVERSE PROBLEM

The inverse problem under consideration here consists of determining the index of refraction of the scattered body from a finite set of N measurements of the scattered field. The l th measurement consists of obtaining the value of the scattered field $u^s(x_l,k_l;v_m)$ at a point x_l exterior to the body, and at a frequency associated with the wavenumber k_l, where the scattered field is produced by an incident field $u^i(x,k_l)$. Each measured scattered field may be produced by a different incident wave. For simplification the notation $u^s_m(x_l)$ will be used for the measured quantity $u^s(x_l,k_l;v_m)$.

The inverse problem can be stated as follows: Find a solution v of the system of N nonlinear complex functional equations;

$$u^s(x_l,k_l;v) - u^s_m(x_l) = 0, \quad l = 1,...,N. \tag{3}$$

This can be placed in a more explicit form. Let v_* represent a (known) comparison body, G_* its Green's function. Then as stated,[1] the above system (3) is equivalent to solving the system ($l = 1,...,N$)

$$u^s_*(x_l,k_l) + k_l^2 \int_D G_*(x_l,y,k_l)[v(y) - v_*(y)] \times u(y,k_l)dy - u^s_m(x_l,k_l) = 0, \tag{4a}$$

where $u(x,k_l)$ must satisfy the integral equation

$$u(x,k_l) = u_*(x,k_l) + k_l^2 \int_D G_*(x,y;k_l) \times [v(y) - v_*(y)]u(y,k_l)dy. \tag{4b}$$

[Here $u^s_*(x_l,k_l)$ represents the scattered field at x_l produced by the same incident wave $u^i(x,k_l)$ on the comparison body v_*.]

III. RESOLUTION CELL

A. Definition

We shall define the set of solutions v of the inverse problem Eq. (3) [or equivalent system (4a) and (4b)] as the resolution cell (solution space). It will be shown that the resolution cell is not an isolated set of points but an infinite-dimensional manifold.

 0022-2488/84/123483-06$02.50

B. Formulation of the problem

Let $v_* = v_m$, then Eq. (4a) reduces to

$$u^s(x_l,k_l;v) - u^s_m(x_l)$$

$$\equiv k_l^2 \int_D G_m(x_l,y;k_l)(v - v_m)u(y,k_l)dy = 0, \tag{5}$$

with $l = 1,2,...,N$, and where $u(x,k_l)$ must satisfy Eq. (4b) with G_* replaced by G_m and v_* by v_m.

It is immediately obvious as expected, that system (5) is satisfied by $v = v_m$. However the existence of other solutions in a region close to and containing v_m can be demonstrated by considering the linearized version of Eq. (5) where $v - v_m$ is sufficiently small so that the term $u(y,k_l)$ in Eq. (5) can be replaced by $u_m(y,k_l)$. Using the notation introduced in the previous paper[1]

$$k_l^2 G_m(x_l,y;k_l)u_m(y,k_l) = H_l(y;v_m) + iH_{l+N}(y;v_m),$$

the linearized version of system (5) can be reduced to the system of $2N$ real equations

$$\int_D H_l(x;v_m)w(x)dx = 0, \quad l = 1,...,2N,$$

where $w = v - v_m$. This has the nonunique solution

$$v - v_m = \mu\varphi^\perp,$$

where $\varphi^\perp$ is an arbitrary function in the space $C_p(D) \cap \mathcal{M}^\perp_m$ where $\mathcal{M}_m$ is the space spanned by $H_k(x;v_m)$, $k = 1,...,2N$.

This suggests that to study solutions of system (5) in a region close to and containing v_m, a solution of the form

$$v_p(x) = v_m(x) + \mu\varphi^\perp(x) + \sum_{k=1}^{2N} c_k H_k(x;v_m) \tag{6}$$

should be taken. Here it is convenient to normalize $\varphi^\perp$ so that

$$\|\varphi^\perp\| = \left(\int_D (\varphi^\perp)^2 dx\right)^{1/2} = 1.$$

By then *fixing* the value of $\varphi^\perp(x)$, the unknown expression (6) contains $2N + 1$ real variables $\mu,c_1,c_2,...,c_{2N}$, and the associated inverse problem reduces to a problem in a space of $2N + 1$ dimensions. With $\varphi^\perp$ a fixed prescribed value, set

$$f_l(\mu;c_1,c_2,...,c_{2N}) = u^s(x_l,k_l;v_p) - u^s_m(x_l), \tag{7}$$

where v_p is given by Eq. (6), then the inverse problem for finding solutions in a region about v_m, consists of solving the N complex nonlinear functional equations

$$f_l(\mu;c_1,c_2,...,c_{2N}) = 0, \quad l = 1,...,N \tag{8}$$

for the $2N + 1$ real variables $\mu,c_1,...,c_{2N}$. The point corresponding to v_m is the origin $\mu = c_1 = \cdots = c_{2N} = 0$. For each choice of $\varphi^\perp$, the corresponding solution of Eq. (8) will give solutions in a prescribed $(2N + 1)$-dimensional space containing v_m.

To solve the complex system for the real variables it is convenient to decompose it into real and imaginary parts by setting

$$f_l(\mu;c_1,...,c_{2N}) = F_l(u;c_1,...,c_{2N}) + iF_{l+N}(\mu;c_1,...,c_{2N}), \tag{9}$$

yielding the system of $2N$ real equations

$$F_l(\mu;c_1,...,c_{2N}) = 0, \quad l = 1,...,2N. \tag{10}$$

With $2N$ real equations and $2N + 1$ real unknown variables, one of the variables can be taken as a parameter and the resulting solution will describe a curve in the $(2N + 1)$-dimensional space. That portion of the curve that is continuous and goes through the origin will be sought. This will then yield the projection of the resolution cell surrounding v_m on the $(2N + 1)$-dimensional space spanned by $\varphi^\perp$ and $\{H_k(x;v_m)\}_{k=1}^{2N}$. It is convenient to take μ as the parameter for the portion of the curve in the neighborhood of the origin, since the linearized solution corresponds to the straight line $c_1 = \cdots = c_{2N} = 0, \mu = \mu$.

C. Solution of $F_l = 0$, for small values of parameter μ

We will use the modified form of Newton's method to solve system (10) for small values of the parameter μ, and will seek the solution such that $c_1 = c_2 = \cdots = c_{2N} = 0$, when $\mu = 0$. We will use the notation that c, $F(\mu;c)$ represent column vectors in R^{2N}, with their transposes given by

$$c^T = [c_1,...,c_{2N}], \quad F(\mu;c)^T = [F_1,...,F_{2N}],$$

and $F_c(\mu;c)$ (the Fréchet derivative of F with respect to c) is the linear operator represented by the matrix with (l,k)th component

$$F_c(\mu;c) = \left\{\frac{\partial F_l}{\partial c_k}\right\}, \tag{11}$$

and $F_{cc}(u;c)$ (the second derivative of F) is the bilinear operator with (l,j,k)th component

$$F_{cc}(\mu;c) = \left\{\frac{\partial^2 F_l}{\partial c_k\, \partial c_j}\right\}. \tag{12}$$

With the above notation, system (10) can be expressed in the compact form

$$F(\mu;c) = 0. \tag{13}$$

With μ as a parameter, we seek a solution of (13), $c = c(\mu)$ such that

$$\lim_{\mu \to 0} c(\mu) = 0.$$

With this in mind it is convenient to take as initial point in the Newton process $c^0 = 0$. Thus the modified Newton iteration procedure will be given by

$$c^0 = 0, c^{n+1} = c^n - \Gamma_0 F(\mu;c^n), \tag{14}$$

where

$$\Gamma_0 = [F_c(\mu;0)]^{-1}. \tag{15}$$

To obtain both an explicit form of the solution and an estimate on the range of $|\mu|$ which insures convergence of the iteration process, we need the following results. From the relation [derived from Eqs. (7) and (9)]

$$F_l(\mu;c) + iF_{l+N}(\mu;c) = u^s(x_l,k_l;v_p) - u^s_m,$$

together with Eq. (6) and the result given in the previous paper[1]

$$\delta u^s(x_l;v_p) = (H_l(v_p) + iH_{l+N}(v_p), \delta v_p),$$

it is seen that the differential of F_l with respect to v_p is given by

$$\delta F_l(\mu;c) = (H_l(v_p), \delta v_p). \tag{16}$$

Hence it follows that

$$\frac{\partial F_l(\mu;c)}{\partial c_k} = (H_l(v_p), H_k(v_m)), \tag{17}$$

$$\frac{\partial^2 F_l(\mu;c)}{\partial c_k\, \partial c_j} = ((H'_l(v_p), H_k(v_m)), H_j(v_m)). \tag{18}$$

In addition, from Eq. (16), the Taylor expansion in μ with $c = 0$ is given by

$$F_l(\mu;0) = F_l(0;0) + \mu(H_l(v_m), \varphi^\perp) + \tfrac{1}{2}\mu^2((H'_l(v_m + \theta\mu\varphi^\perp), \varphi^\perp), \varphi^\perp), \quad 0<\theta<1.$$

Using the result that $F_l(0,0) = 0$, and $\varphi^\perp \perp \mathcal{M}_m$, the above simplifies to

$$F_l(\mu;0) = \tfrac{1}{2}\mu^2((H'_l(v_m + \theta\mu\varphi^\perp), \varphi^\perp), \varphi^\perp). \tag{19}$$

Thus for small values of μ, we have to the leading term

$$F_l(\mu,0) \sim \tfrac{1}{2}\mu^2((H'_l(v_m), \varphi^\perp), \varphi^\perp). \tag{20}$$

To obtain the leading terms in μ of the inverse matrix Γ_0, we note that from the Taylor expansion for the right-hand side of Eq. (17) with $c = 0$, we obtain

$$\frac{\partial F_l}{\partial c_k} = H_{lk}(v_m) + A_{lk}(\mu), \tag{21}$$

where $H_{lk}(v_m) = (H_l(v_m), H_k(v_m))$,

$$A_{lk}(\mu) = \mu((H'_l(v_m + \mu\theta_1\varphi^\perp), H_k(v_m)), \varphi^\perp), \tag{22}$$

where $0<\theta_1<1$. It is thus seen that when $H = \{H_{ij}(v_m)\}$ is nonsingular,

$$\Gamma_0 = [I + H^{-1}A(\mu)]^{-1} H^{-1}, \tag{23}$$

where $A(\mu)$ is the matrix with coefficients $A_{lk}(\mu)$. For small μ, it is easily seen that $A_{lk} \sim O(\mu)$, hence

$$\Gamma_0 \sim [I + O(\mu)]H^{-1}(v_m). \tag{24}$$

Combining results of Eqs. (14) and (24) it is seen that the leading term in μ of the solution c of system (13) is given by the first iterate c^1, yielding

$$c \sim H^{-1}(v_m)F(\mu;0), \tag{25}$$

where the $F_l(\mu;0)$ are given by Eq. (20). Thus it is seen that $c(\mu) \sim O(\mu^2)$.

Recall that the solution of the linearized problem is given by

$$v = v_m + \mu\varphi^\perp,$$

thus we see that the nonlinear correction to this is of order μ^2. The neighboring solution to v_m of the order μ^2 is given explicitly by

$$v = v_m + \mu\varphi^\perp - \tfrac{1}{2}\mu^2 H^{-1}(v_m)p\cdot\mathbf{H}(v_m), \tag{26}$$

where p is a vector with components

$$p_l = ((H'_l(v_m),\varphi^\perp),\varphi^\perp). \tag{27}$$

We now want to get an estimate for the range of μ for which Newton process (14) converges. As a preliminary we need the following notation and definitions.

For the functions $H_k(x;v)$ and $H'_k(x,y;v)$ we use the respective $\mathcal{L}_2(D)$ and $\mathcal{L}_2(D\times D)$ norms,

$$\|H_k(v_m)\|^2 = \int_D H_k^2(x;v_m)dx,$$

$$\|H'_k(v_m)\|^2 = \int_{D\times D} [H'_k(x,y;v_m)]^2\, dx\, dy,$$

and for a vector η in R^{2N} the norm

$$\|\eta\|_2 = \left(\sum_{j=1}^{2N} \eta_j^2\right)^{1/2}.$$

Set

$$K_1 = \left(\sum_{k=1}^{2N} \|H_k(v_m)\|^2\right)^{1/2}, \tag{28}$$

$$K_2(\mu;c) = \left(\sum_{k=1}^{2N} \|H'_k(v_p)\|^2\right)^{1/2}, \tag{29}$$

where we recall v_p is given by Eq. (6). We will assume that the positive matrix $H(v_m)$ is nonsingular, and set

$$\lambda_M = \text{smallest eigenvalue of } H(v_m). \tag{30}$$

Then set

$$\mu_0 = \lambda_M(K_1K_2(0;0))^{-1}, \tag{31}$$

$$r = \tfrac{1}{2}\mu_0 K_1^{-1},$$

$$K_3 = \max_{\substack{0<|\mu|<\mu_0 \\ |c|<r}} K_2(\mu;c). \tag{32}$$

We can now state the result (with proof given in Appendix).

Theorem: For the parameter μ in the range $|\mu| \leqslant \tfrac{1}{2}\mu_0 K_0(0;0)/K_3$. Newton's iteration process Eq. (14) converges to a solution c_{**} in the ball $\|c_{**}\|_2 < r$.

By taking all possible values of $\varphi^\perp$, the existence of the resolution cell in a region about v_m, contained in a neighborhood $\|v - v_m\| \sim O(\lambda_m)$ can be shown. Furthermore, the region can be extended by repeating the procedure with v_m replaced by a neighboring value in the resolution cell. The only problem with this continuation occurs when one approaches a singular point where λ_m is zero. This is briefly discussed next.

D. Solution in the singular case

For completeness a brief formal treatment of the singular case [when a point v_m in the resolution cell has a singular matrix $H(v_m)$] is treated. It will be demonstrated that the resolution cell is not bounded or terminated by the singular points. Since the singularity of the matrix $H(v_m)$ implies that the set $H_k(x;v_m)$, $k = 1,...,2N$ is linearly dependent, expression (6) for a point in the resolution cell adjacent to v_m will have to be modified. Let

$$\text{Rank } H(v_m) = p$$

and assume that the $H_k(x;v_m)$ are ordered so that $H_1,...,H_p$ are linearly independent, and let the dependency relationships among the H_k be given by

$$\sum_{k=1}^{2N} \alpha_k^r H_k(x;v_m) = 0, \quad r = 1,...,2N-p. \tag{33}$$

Set[7]

$$\sum_{k=1}^{2N} \alpha_k^r H'_k(x,y;v_m) = a_r(x,y), \quad r = 1,...,2N-p. \tag{34}$$

Then pick out a set of $2N - p + 1$ functions $\hat{H}_{p+1},...,\hat{H}_{2N}(x)$,

and $\varphi^{\perp}(x)$ such that they have the following properties: (i) $\hat{H}_{p+1},\ldots,\hat{H}_{2N}$ and $\varphi^{\perp}$ are orthogonal to $H_k(x;v_m), k=1,\ldots,p$; (ii) the $2n-p$ square matrix with elements $((a_i,\varphi^{\perp}),\hat{H}_k)$ is nonsingular; and (iii) $((a_i,\varphi^{\perp}),\varphi^{\perp})=0, i=1,\ldots,2N-p$. Then look for a solution in the resolution cell adjacent to v_m in the form

$$v = v_m + \mu\varphi^{\perp} + \sum_{k=1}^{p} c_k H_k(x;v_m) + \sum_{k=p+1}^{2N} c_k \hat{H}_k(x), \tag{35}$$

where μ is a small parameter, and the real constants c_k are to be found in terms of μ. Now the system of equations (5) become, for $v-v_m$ small,

$$(H_l(v_m),v-v_m) + \tfrac{1}{2}((H_l'(v_m),v-v_m),v-v_m) + \cdots = 0, \tag{36}$$

where $l=1,\ldots,2N$. The insertion of expression (35) into (36), combined with the use of properties (i)–(iii) yields

$$\sum_{k=1}^{p} H_{lk}c_k + \frac{1}{2}\mu^2((H_l',\varphi^{\perp}),\varphi^{\perp}) + \mu\sum_{k=1}^{p}((H_l',\varphi^{\perp}),H_k)c_k + \mu\sum_{k=p+1}^{2N}((H_l',\varphi^{\perp}),\hat{H}_k)c_k + O(c_k^2) = 0, \tag{37}$$

where $l=1,\ldots,2N$. Employ the linear dependency relationships [Eqs. (33) and (34)] and the properties (i) and (iii) to obtain the system of $2N-p$ equations

$$\mu\sum_{k=p+1}^{2N}((a_r,\varphi^{\perp}),\hat{H}_k)c_k = -\mu\sum_{k=1}^{p}((a_r,\varphi^{\perp}),H_k)c_k + O(c_k^2), \tag{38}$$

where $r=1,\ldots,2N-p$. Now because of property (ii) the coefficients $c_k, k=p+1,\ldots,2N$ can be solved in terms of c_k for $k=1,\ldots,p$, where the higher-order terms $O(c_k^2)$ are neglected. The interest here is in the solution where the c_k are close to zero. The solution for c_k, $k=p+1,\ldots,2N$ can then be inserted back into system (37) with $l=1,\ldots,p$ resulting in a system of p equations in p unknowns c_k, $k=1,\ldots,p$.

For small values of μ, the solution is given by

$$c_l = -\frac{\mu^2}{2}\sum_{k=1}^{p}\tilde{H}_{lk}((H_k',\varphi^{\perp}),\varphi^{\perp}) + O(\mu^3), \tag{39}$$

for $l=1,\ldots,p$. Here $\tilde{H}_{lk}$ is the (l,k)th element of the $p\times p$ inverse matrix to $H_{lk}=(H_l,H_k)$.

A rigorous treatment and analysis of Newton's method of singular points is given in Refs. 8 and 9.

E. Intersection of the resolution cell with a subspace of dimension 2N

In order to further delineate the resolution cell restrict v to lie in a prescribed $2N$-dimensional subspace $\mathcal{M}_{\varphi}$ of $\mathcal{L}_2(D)$, with basis $\{\varphi_j\}_{j=1}^{2N}$. Then v will take on the form

$$v = \sum_{j=1}^{2N} c_j\varphi_j(x), \tag{40}$$

and the c_j's will be chosen so that v and v_m have the same scattered field at the N pairs (x_l,k_l), i.e.,

$$u^s(x_l,k_l;v) - u_m^s(x_l,k_l) = 0, \quad l=1,\ldots,N.$$

With the notation $c^T=[c_1,\ldots,c_{2N}]$ and

$$f_l(c) = F_l(c) + iF_{l+N}(c) = u^s\left(x_l,k_l;\sum_{j=1}^{2N}c_j\varphi_j\right) - u_m^s(x_l,k_l),$$

the above system of equations reduces to a system of $2N$ real equations expressed in vector form

$$F(c)=0,$$

where $F^T=[F_1,\ldots,F_{2N}]$. With the derivative of $F(c)$ being given by the matrix with (l,k)th component $\partial F_l/\partial c_k$ it can be shown that

$$F'(c) = \left[\frac{\partial F_l}{\partial c_k}\right] = (H_l(v),\varphi_k). \tag{41}$$

Define $\mathcal{M}_v$ as the subspace spanned by $\{H_l(v)\}_{l=1}^{2N}$, and let $\mathcal{S}$ be a region of $\mathcal{M}_{\varphi}$ such that $v\in\mathcal{S}$ when (i) $\{H_l(v)\}_{l=1}^{2N}$ are linearly independent, and (ii) the only vector in $\mathcal{M}_v$ orthogonal to $\mathcal{M}_{\varphi}$ is zero. It then follows that for $v=\Sigma_{j=1}^{2N}c_j\varphi_j$ in $\mathcal{S}$, $F'(c)$ is invertible and by the implicit function theorem, the solution of $F(c)=0$ is a set of isolated points. Thus it is seen that on restricting v to lie in $2N$-dimensional space, the solution of the inverse problem (when v is in $\mathcal{S}$) is an isolated set of points lying in the resolution cell. Different subspaces $\mathcal{M}_{\varphi}$ will give rise to different point solutions.

F. Summary of properties of resolution cell

It has been shown that the resolution cell (solution space) is not an isolated set of points but an infinite-dimensional manifold. Its intersection with a $2N$-dimensional subspace (with basis $\{\varphi_j\}_{j=1}^{2N}$) is a set of isolated points in a region where the matrix with (i,j)th element (H_i,φ_j) is nonsingular. It is not known, however, whether the resolution cell is a single connected region or a set of connected regions.

IV. STRUCTURAL STABILITY

A. Stability condition

Nonuniqueness is not serious if the set of solutions are isolated points. Here, restrictions on the initial choice used in any iterative procedure, and the design of the experiment (the selection of measured data) will determine which particular solution is obtained. The more serious problem is the case where the resolution cell is an infinite-dimensional manifold. One needs additional criteria to select the proper solution or solutions. Without using *a priori* knowledge, one needs a condition that is intrinsic to the process. A natural condition in the inverse problem wth sparse data is to select stable solutions. Such a solution has the property that small changes in scattered data produce small changes in the solution. If v_m is a solution corresponding to data $u_m^s(x_l,k_l)$, $l=1,\ldots,N$, and δu_m^s represents a small change in data, then the change in solution δv satisfies the relation

$$u^s(x_l,k_l;v_m+\delta v) - u_m^s(x_l,k_l) - \delta u_m^s = 0,$$

$l=1,\ldots,N$. On linearizing the system and decomposing the complex quantity δu_m^s into real and imaginary parts, $\delta u_m^s(x_l,k_l)=\Delta_l + i\Delta_{l+N}$, one obtains the system of $2N$ real equations

$$(H_l(v),\delta v) = \Delta_l .$$

From the previous paper[1] the least square solution of the system has the property that

$$\|\delta v\|^2 = \sum_{l,k=1}^{2N} \Delta_l \tilde{H}_{lk} \Delta_k,$$

where $\tilde{H}_{lk}$ are the elements of the inverse matrix $H^{-1}(v)$, with $H(v) = \{H_{ij}\}$. Thus for small $\|\delta v\|$, $\|H^{-1}(v)\|_2$ must be small as possible. As a result, one can say the most stable solution is that for which

$$\left.\begin{aligned} &\text{Min}\|H^{-1}(v)\|_2, \\ &u^s(x_l,k_l;v) - u^s_m(x_l,k_l) = 0, \\ &\quad l = 1,2,...,N. \end{aligned}\right\} \text{I}$$

Another possible condition for stability, although not as practical to implement, is to look at the conditioning[10] associated with the matrix $H(v)$, and require a solution which minimizes $\|H^{-1}\|_2\|H\|_2$.

B. Stationary point for λ_M

We want to briefly examine the points where $\|H^{-1}\|_2$ is a minimum or, what is equivalent, where λ_M (the smallest eigenvalue of H) is a maximum.

Let the eigenvalues of H be ordered so that $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_{2N}$. Assume that the smallest eigenvalue of H has multiplicity p so that $\lambda_1 = \lambda_2 = \cdots = \lambda_p = \lambda_M$. Let ψ_l be the eigenvector (with components ψ^j, $j = 1,...,2N$) corresponding to λ_j and let $\{\psi_l\}$ form an orthonormal set.

With the matrix $H(v)$ and $\lambda_l(v)$ expanded in Taylor series in the variable δv,

$$H + \delta H + \tfrac{1}{2}\delta^2 H + \cdots,$$

$$\lambda_l + \delta\lambda_l + \tfrac{1}{2}\delta^2\lambda_l + \cdots,$$

it can be shown from well-known perturbation theory,[11] that

$$\delta\lambda_l = \psi_l \cdot \delta H \psi_l. \tag{42}$$

Since the (i,j)th component of the matrix H is the scalar product $H_{ij} = (H_i,H_j)$ it follows that the (i,j)th component of the matrix δH is

$$(\delta H)_{ij} = (\delta H_i,H_j) + (H_i,\delta H_j).$$

Using the notation[1]

$$\delta H_j = \int_D H'_j(x,y;v)\delta v(y)dy,$$

to define the functions

$$c_l(x;v) = \sum_{j=1}^{2N} \psi^j_l H_j(x;v), \tag{43}$$

$$a_l(x,y;v) = \sum_{j=1}^{2N} \psi^j_l H'_j(x,y;v), \tag{44}$$

it is seen that

$$\delta\lambda_l = 2(\mathfrak{U}_l c_l,\delta v),$$

where $\mathfrak{U}_l$ is the integral operator with kernel $a_l(x,y;v)$. A necessary condition for λ_M to be a maximum is that $\delta\lambda_l = 0$, for $l = 1,..., p$, for all values of v and δv such that v and $v + \delta v$ is in the resolution cell. From Sec. III B, it is seen then that δv must be orthogonal to the subspace spanned by $\{H_j(v)\}_{j=1}^{2N}$. Let $\mathfrak{B}$ be the projection operator on this space. Then $\delta\lambda_l$, $l = 1,..., p$ must vanish for all δv of the form $\delta v = (\mathfrak{I} - \mathfrak{B})\delta q$ for any δq in $\mathscr{L}_2(D)$. It then follows that a necessary condition for λ_M to be a maximum is that

$$(\mathfrak{I} - \mathfrak{B})\mathfrak{U}_l c_l \equiv 0, \quad l = 1,..., p. \tag{45}$$

It should be noted that $c_l(x;v) \equiv 0$ iff $\lambda_l \equiv 0$. This is easily seen, since $c_l \equiv 0$ implies that $\{H_j\}_{j=1}^{2N}$ is a linear dependent set, hence the matrix $H_{ij} = (H_i,H_j)$ is singular. Thus a necessary condition for λ_M to be a maximum is that

$$(\mathfrak{I} - \mathfrak{B})\mathfrak{U}_l c_l = 0, \quad \|c_l\| \neq 0, \quad l = 1,..., p. \tag{46}$$

One requires the additional condition that $\delta^2\lambda_M > 0$ to guarantee a local maximum. However without this condition, it is seen that system (46) coupled with the finite set (3) reduces the number of possible solutions.

To clarify this last statement consider the case (used in numerical computations) where v is restricted to be in a finite-dimensional subspace of dimension M where $M \gg 2N$. In this case the requirement that δv be orthogonal to $\{H_j\}_{j=1}^{2N}$ restricts δv to lie in a $(M - 2N)$-dimensional space. It is seen that when the smallest eigenvalue has multiplicity 1 ($p = 1$), the system $\delta\lambda_1 = 0$ reduces to a system of $M - 2N$ equations. When this is coupled with the set of $2N$ real equations, Eq. (3) produces a total of M nonlinear real equations in M unknowns, which yields isolated solutions at points (where the derivative does not vanish).

C. Structural stability of inverse procedures

Here the structural stability of the descent process developed in the previous paper[1] is examined. First note that the problem of solving the system of complex equations

$$u^s(x_l,k_l;v) - u^s_m(x_l,k_l) \equiv B_l(v) + iB_{l+N}(v) = 0,$$
$$l = 1,...,N$$

is equivalent to minimizing the real quadratic form

$$\sum_{i,j=1}^{2N}\sum B_i(v)T_{ij}B_j(v),$$

where $\{T_{ij}\}$ is a given positive definite matrix. Thus system I giving stable solutions is equivalent to

$$\left.\begin{aligned} &\text{Min} \sum_{i,j=1}^{2N}\sum B_i(v)T_{ij}B_j(v), \\ &\text{Min}_{\|\theta\|_2=1} \sum_{i,j=1}^{2N}\sum \theta_i\tilde{H}_{ij}\theta_j. \end{aligned}\right\} \text{I(a)}$$

The procedure developed in the previous paper[1] combines the two minimization steps making it more practical. There the descent procedure is applied to the following minimization problem

$$\text{Min} \sum_{i,j=1}^{2N}\sum B_i(v)\tilde{H}_{ij}(v)B_j(v). \quad \text{II}$$

However since $\|B_i(v)\| \neq 1$, the stability effect is not as pronounced as $\|B_i(v)\|$ tends to zero. For this and other reasons, the descent process is not carried out all the way but is terminated when the approximate solution v is in the linear region of a point in the resolution cell. At this point, other

various techniques could be imposed such as that of Backus and Gilbert[2] to get the smoothest solution.

It is clear however that the conjugate gradient and other methods applied to the minimization of $\Sigma_{i=1}^{2N} B_i^2(v)$ are unstable, and are only useful in the case of a large data base when v may be satisfactorily represented by a point in a $2N$-dimensional subspace. For the latter situation it is expected that the conditioning of the matrix H will tend to get worse as N increases, hence there is some measurement number N, such that one can take as subspace dimension $M = 2N$ or if N is large enough $M < 2N$.

D. Design of experiment

In order for the problem to be well posed an additional condition or constraint has to be imposed to select a particular solution from the isolated point set. This is achieved by proper design of experiment and initial choice of v used in the iteration scheme. Although the actual requirements still remain to be completely formulated and rigorously verified, some conjectures on them can be made based on physical reasoning (verified by computational studies). In the design of the experiment at least one of the measurements should be made at a low enough frequency so that the Born approximation can be made. A suitable initial choice for v in the iteration scheme is to take a value which is constant over D, where the constant v_{Born} is the value obtained from the Born approximation. The remaining measurements should be made at frequencies and positions that are sufficiently different so that the matrix H for the body is not too singular. The precise quantification of this remains to be done.

ACKNOWLEDGMENT

The research reported herein was supported through the Office of Naval Research Grant No. N14-83-K-6038.

APPENDIX: PROOF OF THEOREM

Here the proof of the following theorem is presented.

Theorem: For the parameter μ in the range $|\mu| \leqslant \frac{1}{2}\mu_0 K_2(0;0)/K_3$, Newton's iteration process [Eq. (14)] converges to a solution c_{**} in the ball $\|c_{**}\|_2 < r$.

Proof: Using Schwarz's inequality for the Hilbert space associated with $\mathscr{L}_2(D \times D)$ and the fact that we set $\|\varphi^\perp\| = 1$, we have

$$|((H_l'(v_p),\varphi^\perp),\varphi^\perp)| \leqslant \|H'(v_p)\|.$$

Hence it follows from Eqs. (29) and (19), that for $|\mu| < \mu_0$,

$$\|F(\mu;0)\|_2 \leqslant \tfrac{1}{2}\mu^2 K_2(\theta\mu;0) \leqslant \tfrac{1}{2}\mu^2 K_3, \tag{A1}$$

where $0 < \theta < 1$.

From Eq. (12) it follows in similar manner that

$$|A_{lk}(\mu)| < |\mu| \|H_l'(v_m + \mu\theta_1\varphi^\perp)\| \|H_k(v_m)\|,$$

$$\sum_{l,k=1}^{2N} |A_{lk}|^2 \leqslant (|\mu| K_2(\mu\theta_1;0) K_1)^2,$$

where $0 < \theta_1 < 1$. Thus we obtain the estimate on the norm of the matrix

$$\|A\|_2 < |\mu| K_2(\mu\theta_1;0) K_1. \tag{A2}$$

It then follows from Eq. (11) that the norm of the inverse matrix satisfies the inequality

$$\|\Gamma_0\|_2 \leqslant \|H^{-1}\|_2 [1 - \|H^{-1}\|_2 \|A\|_2]^{-1}.$$

From Eq. (A2) it is seen that

$$\|H^{-1}\|_2 \|A\|_2 < \rho,$$

where

$$\rho = (|\mu|/\lambda_M) K_1 K_3, \tag{A3}$$

hence

$$\|\Gamma_0\|_2 \leqslant (1/\lambda_M)(1-\rho)^{-1}. \tag{A4}$$

To get an estimate for $\|F_{cc}(\mu;c)\|_2$ for $\|c\| < r$, and $|\mu| < \mu_0$, we note that from Eq. (18)

$$\left| \frac{\partial^2 F_l}{\partial c_k \, \partial c_j}(\mu;c) \right| \leqslant \|H_l'(v_p)\| \|H_k(v_m)\| \|H_j(v_m)\|,$$

hence

$$(\|F_{cc}(\mu;c)\|_2)^2 \leqslant \sum_{j,k,l=1}^{2N} \left| \frac{\partial^2 F_l}{\partial c_k \, \partial c_j}(\mu;c) \right|^2 \leqslant K_1^4 K_2^2(\mu;c) \leqslant K_1^4 K_3^2. \tag{A5}$$

Using the notation of Vainberg[12] we have

$$\|\Gamma_0 F(\mu;0)\|_2 \leqslant \eta = \tfrac{1}{2}[\mu^2 K_3/\lambda_M(1-\rho)], \tag{A6}$$

$$\|\Gamma_0 F_{cc}(\mu;c)\|_2 \leqslant K = K_1^2 K_3/\lambda_M(1-\rho), \tag{A7}$$

$$h = \eta K = \tfrac{1}{2}(\rho/(1-\rho))^2. \tag{A8}$$

Thus for $|\mu| \leqslant \frac{1}{2}\mu_0 K_2(0,0)/K_3$, it follows from Eq. (A3) that $\rho < \frac{1}{2}$, and $h < \frac{1}{2}$. Hence from the Theorem (27.6) of Vainberg,[12] the Newton process converges to a solution c_{**} in the ball

$$\|c_{**}\|_2 \leqslant [(1 - \sqrt{1-2h})/h]\eta = r_0.$$

It can be shown that for the range of μ specified above,

$$r_0 \leqslant 2\eta = \frac{2\mu^2 K_3}{\lambda_M} \leqslant \frac{2\mu_0 K_3}{K_1 K_2(0,0)} \left(\frac{\mu}{\mu_0}\right)^2 < \frac{1}{2}\frac{\mu_0}{K_1} = r.$$

In addition from Vainberg, the solution is unique in the ball $\|c\|_2 < \text{Min}(r, r_1)$, where

$$r_1 = [(1 + \sqrt{1-2h})/h]\eta.$$

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A rule for the total number of topologically distinct Feynman diagrams

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(Received 24 January 1984; accepted for publication 4 May 1984)

A rule for the total number of topologically distinct Feynman diagrams is presented for the ground state of a system of many identical particles interacting via a two-body potential.

PACS numbers: 03.65.Db, 02.40. + m

I. INTRODUCTION

The idea of quantization comes from wave–particle duality. One starts with the classical equations of motion of a given system and quantizes them by treating the dynamical variables as operators and imposing a specific algebra. This procedure is called particle or field quantization, depending on whether it is applied to classical particles or classical fields. Given that field quantization leads to a many-particle description, it is then natural to ask whether one can consider a field-quantized description of many-particle systems. This is possible, and the procedure is called second quantization.

Although the concept of second quantization is essential in a relativistic theory where one wants to allow the total number of particles in the system to be a variable, in nonrelativistic problems it becomes a very useful technique when one takes into account the statistics of the many-particle system under study, without the need for symmetrizing or antisymmetrizing products of single-particle wave functions. Only a few cases can be solved exactly[1] with the second-quantized Hamiltonian, and often after a canonical transformation has had to be performed. In general, one must resort to approximate methods in which part of the Hamiltonian is considered exactly soluble and the remainder is treated as a perturbation. In many-particle physics the perturbation expansion becomes quite cumbersome, but can be written in an elegant and concise form using the language of Feynman diagrams.[2] The main utility of such diagrams lies in the fact that one can represent graphically various terms in a particular series expansion, give a physical interpretation to them, and easily perform sums of an *infinite* class of perturbation terms. In fact, in many-body theory the interaction between particles is not necessarily weak, so that a perturbation theory in which one considers only the first term, or even the first few terms, will not give satisfactory results. Feynman diagrams have proved useful in developing techniques by which we can pick out from the infinite set of all terms of the perturbation expansion an infinite subset of terms which are believed, on physical grounds, to be more important, and sum them up to arrive at a reasonable approximation for the quantity to be calculated. Moreover, as we want to show in this paper, the number of terms that need be considered if one wants to compute all the terms up to order n in the perturbation expansion grows so rapidly that it becomes necessary to stop at a very low value of n. In Sec. II we shall briefly review the diagrammatic technique, and in Sec. III we shall give a rule to determine, at each order n in the perturbation expansion, the total number of topologically distinct diagrams one should consider to compute the ground-state Green's function of a system of many fermions interacting via a two-body potential.

II. GREEN'S FUNCTION AND DIAGRAMMATIC REPRESENTATION

The field operator for a many-particle system in the Heisenberg picture can be written as

$$\hat{\psi}_\alpha(\mathbf{x}) = e^{iHt}\hat{\psi}^S_\alpha(\mathbf{x})e^{-iHt}, \tag{1}$$

in terms of the field operator in the Schrödinger picture given by

$$\hat{\psi}^S_\alpha(\mathbf{x}) = \sum_{\mathbf{k}} \psi_{\mathbf{k}\alpha}(\mathbf{x})\hat{c}_{\mathbf{k}\alpha}. \tag{2}$$

Here H is the total Hamiltonian, $\psi_{\mathbf{k}\alpha}(\mathbf{x})$ is the single-particle wave function, and $\hat{c}_{\mathbf{k}\alpha}$ is the annihilation operator for the state $(\mathbf{k}\alpha)$, where $\mathbf{k}$ represents the momentum and α represents a spin component. If $|\psi_0\rangle$ is the exact Heisenberg normalized ground state, then the single-particle Green's function at zero temperature can be defined as[3]

$$iG_{\alpha\beta}(x,y) = \langle\psi_0|T\left[\hat{\psi}_\alpha(x)\hat{\psi}^\dagger_\beta(y)\right]|\psi_0\rangle, \tag{3}$$

where $x \equiv (\mathbf{x},t_x)$, $y \equiv (\mathbf{y},t_y)$, and T is the time-ordering operator. Here $G_{\alpha\beta}$ contains observable properties of great interest, for from it one can compute expectation values of any single-particle operator in the ground or excited state of the system.

The construction of the Green's function for a nontrivial physical system, however, is a formidable job, and a general approach is the use of perturbation theory which splits the Hamiltonian as

$$H = H_0 + V, \tag{4}$$

where the problem for H_0 is assumed to be already solved exactly. Perturbation techniques are most conveniently applied in the interaction picture, and for a many-fermion system with a two-body potential $V(\mathbf{x}_1,\mathbf{x}_2)$, the Green's function is given by

$$\begin{aligned} iG_{\alpha\beta}(x,y) = \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n \\ \times\langle\phi_0|T\left[\tilde{V}(t_1)\cdots\tilde{V}(t_n)\hat{\tilde{\psi}}_\alpha(x)\hat{\tilde{\psi}}^\dagger_\beta(y)\right]|\phi_0\rangle \\ \times\left[\langle\phi_0|\tilde{U}(+\infty,-\infty)|\phi_0\rangle\right]^{-1}, \end{aligned} \tag{5}$$

where $|\phi_0\rangle$ is the unperturbed ground state, $\tilde{U}(\infty,-\infty)$ is the evolution operator, and the tildes remind us that the operators are in the interaction picture. The two-body potential can be expressed in terms of field operators as

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$$V(\mathbf{x}_1,\mathbf{x}_2)=\sum_{\substack{\lambda\lambda'\\ \mu\mu'}}\frac{1}{2}\int d^3x_1\, d^3x_2\, V_{\lambda\lambda',\mu\mu'}(\mathbf{x}_1,\mathbf{x}_2)\times\tilde{\hat{\psi}}^{\dagger}_{\lambda}(\mathbf{x}_1)\tilde{\hat{\psi}}^{\dagger}_{\mu}(\mathbf{x}_2)\tilde{\hat{\psi}}_{\mu'}(\mathbf{x}_2)\tilde{\hat{\psi}}_{\lambda'}(\mathbf{x}_1). \tag{6}$$

One can then see that in order to compute the nth order contribution to $G_{\alpha\beta}$, one must find the expectation value in the unperturbed ground state of the time-ordered product of $4n+2$ creation and annihilation operators of the form

$$\langle\phi_0|T\Big[\underbrace{\tilde{\hat{\psi}}^{\dagger}\cdots\tilde{\hat{\psi}}}_{4n}\tilde{\hat{\psi}}_{\alpha}(x)\tilde{\hat{\psi}}^{\dagger}_{\beta}(y)\Big]|\phi_0\rangle. \tag{7}$$

Using Wick's theorem,[4] given that vacuum expectation values are computed, one arrives at the conclusion that only the fully contracted terms contribute.

It is possible to give a pictorial representation of each of these terms by means of Feynman diagrams. The only diagrams which need be considered are the connected ones, because the disconnected ones are canceled at any order[5] by the vacuum polarization graphs which originate with the denominator $\langle\phi_0|\tilde{U}(\infty,-\infty)|\phi_0\rangle$ appearing in Eq. (5). The equation can then be written as

$$iG_{\alpha\beta}(x,y)=\sum_{n=0}^{\infty}(-2i)^n\int_{-\infty}^{\infty}dt_1\cdots\int_{-\infty}^{\infty}dt_n\times\langle\phi_0|T\,[\tilde{V}(t_1)\cdots\tilde{V}(t_n)\tilde{\hat{\psi}}_{\alpha}(x)\tilde{\hat{\psi}}^{\dagger}_{\beta}(y)]\,|\phi_0\rangle', \tag{8}$$

where the prime stands for "connected and topologically distinct." For example, for $n=1$ there are only two such diagrams which are displayed in Fig. 1. In general, at the nth order each topologically distinct graph contributes $n!$ times.

III. THE RULE

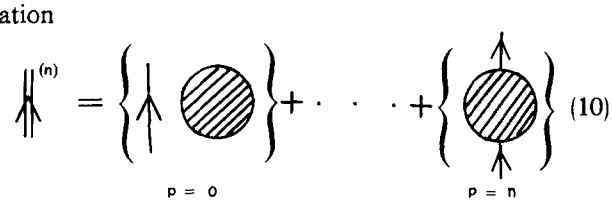
We are now in a position to present a rule for the total number of topologically distinct diagrams that can be drawn for a system of many identical particles interacting via a two-body potential. The number of fully contracted terms which are generated by the expectation value (7) is

$$N(n)=C(n)+D(n)=(2n+1)!, \tag{9}$$

where $C(n)$ is the number of connected terms, $D(n)$ is the number of disconnected terms, and n is the order of approximation in the perturbation expansion. We now give the following definition.

Definition: A term is said to belong to the class of order p if p is the total number of interactions appearing in the connected part of the term which contains $\psi_{\alpha}(x)$ and $\psi^{\dagger}_{\beta}(y)$.

Clearly then (1) $0\leqslant p\leqslant n\rightarrow n+1$ classes; and (2) the above definition makes a partition of the set of $N(n)$ terms into disjoint classes. Graphically this can be expressed by the equation



(10)

for the nth-order Green's function, where the curly brackets contain the whole terms belonging to the class p.

Indicating by $d_p(n)$ the number of nth-order terms belonging to the class p, we can write

$$d_n(n)\equiv C(n)=N(n)-\sum_{p=0}^{n-1}d_p(n). \tag{11}$$

Denoting a free Green's function by a set of parentheses (,), each of which contains a pair of 4-space coordinates, we can write a generic term of order n belonging to class p as

$$\underbrace{(x,\ )(\ ,\ )\cdots(\ ,\ )(\ ,y)}_{2p+1}\underbrace{(\ ,\ )\cdots(\ ,\ )}_{2(n-p)}$$

and

$$\begin{aligned}d_p(n)&=\begin{bmatrix}\text{number of terms of order } p\\ \text{belonging to class } p\end{bmatrix}\\&\times\begin{bmatrix}\text{number of permutations of}\\ 2(n-p)\text{ internal coordinates}\end{bmatrix}\\&\times\begin{bmatrix}\text{number of ways of connecting}\\ n\text{ interactions in groups of } p\end{bmatrix}\\&=C(p)[2(n-p)]!\binom{n}{p}\\&=\Big\{(2p+1)!-\sum_{k=0}^{p-1}d_k(p)\Big\}[2(n-p)]!\binom{n}{p},\end{aligned} \tag{12}$$

$$C(n)=(2n+1)!-\sum_{p=0}^{n-1}\Big\{[2(n-p)]!\binom{n}{p}\Big[(2p+1)!-\sum_{k=0}^{p-1}d_k(p)\Big]\Big\}. \tag{13}$$

We note that Eq. (12) gives the number of disconnected diagrams of order n and class p in terms of the number of disconnected diagrams of lower order, provided that $p<n$. For $p=n$, the equation simply says that $d_n(n)\equiv C(n)$ is given by subtracting the total number of disconnected diagrams from the total number of diagrams. For this reason we give both equations, (12) and (13): the latter gives $C(n)$ in terms of $d_k(p)$ with $p<n$.

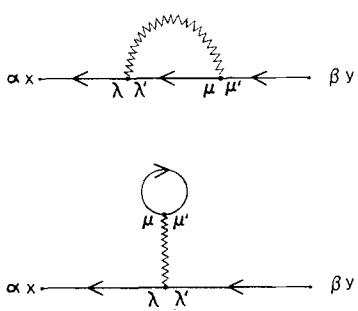


FIG. 1. The two distinct Feynman diagrams for the case $n=1$ in Eq. (7).

TABLE I. Total number $F(n)$ of connected topologically distinct Feynman diagrams.

n	$F(n)$
0	1
1	2
2	10
3	74
4	706
5	8 162
6	110 410
7	1708 391

TABLE II. Each term gives $d_p(n)$. The coefficients $C(p)$ are obtained by subtracting the sum of the first p terms of the $(p+1)$-th row from $(2p+1)!$

n \ P	0	1	2	3	4
0	1				
1	$2!\binom{1}{0}$	$C(1)$			
2	$4!\binom{2}{0}$	$C(1)2!\binom{2}{1}$	$C(2)$		
3	$6!\binom{3}{0}$	$C(1)4!\binom{3}{1}$	$C(2)2!\binom{3}{2}$	$C(3)$	
4	$8!\binom{4}{0}$	$C(1)6!\binom{4}{1}$	$C(2)4!\binom{4}{2}$	$C(3)2!\binom{4}{3}$	$C(4)$

In order to obtain topologically distinct diagrams, we note that (1) the number of permutations of n interactions is $n!$; and (2) the number of ways to interchange the coordinates in each interaction is given by

$$\sum_{k=0}^{n}\binom{n}{k}=2^n.$$

The number of connected topologically distinct Feynman diagrams for a many-fermion system interacting via a two-body potential is thus

$$F(n)=C(n)/n!2^n, \tag{14}$$

which is tabulated in Table I for values of n up to 7.

It is possible to construct a triangle which gives the number $C(n)$ for each n according to Eq. (11), as shown by the diagonal elements in Table II. This triangle is shown numerically below:

1				
2	4			
24	16	80		
720	288	480	3 552	
40 320	11 520	11 520	28 416	271 104.

From Table I for the values of $F(n)$, we see that the number of topologically distinct diagrams grows rapidly. It is now clear that any approach whereby one computes perturbation expansion up to a given order n becomes impractical even for small values of n. Thanks to the computing facilities currently available, one might still want to compute for a given system all the terms in the perturbation expansion until convergence is achieved.[6] However, in the application of perturbation theory to very large quantum systems, i.e., systems with large spatial dimensions and many degrees of freedom (like in quantum field theory, solid-state physics, theory of real gases, and nuclear structure), one encounters difficulties which are associated with the fact that even small perturbations produce large changes in the energies and eigenfunctions of the whole system, because of the occurrence of terms containing high powers of the volume in the perturbation expansion of physical quantities. As a result, one often has to face the problem of an extremely bad convergence of the series. Therefore, the diagrammatic approach is, in general, totally different: one looks for suitable classifications of the various terms and retains only the most important classes. For example, in Dyson's equation[7] one is able to take into account, at any order of approximation for the proper self-energy, an infinite number of terms appearing in Eq. (5) by computing only a finite number of self-energy insertions.

ACKNOWLEDGMENTS

This research was supported in part by the National Science Foundation under Grants CHE-8022874 and CHE-8320185 and the Air Force Office of Scientific Research (AFSC), United States Air Force, under Grant AFOSR-82-0046. FB thanks the University of Rochester for an Elon Huntington Hooker Graduate Fellowship (1983–84), and the Italian CNR for financial support. TFG acknowledges the Camille and Henry Dreyfus Foundation for a Teacher–Scholar Award (1975–84) and the John Simon Guggenheim Foundation for a Fellowship (1983–84).

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Summation of strongly divergent perturbation series

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(Received 10 January 1984; accepted for publication 25 April 1984)

A new method for summing strongly divergent perturbation series is presented. It is based on the change of the power series into a convergent sequence by means of an order-dependent mapping obtained from a simple scaling relation. The perturbation expansions for a one-dimensional integral and for the ground states of the anharmonic oscillator and of the linear confining potential model are accurately summed in the most unfavorable strong-coupling limit.

PACS numbers: 03.65.Ge, 02.30.Lt,

I. INTRODUCTION

Perturbation series with poor convergence properties proved to be the rule rather than the exception in quantum and field theory. Due to this fact, summability procedures are of utmost importance. Strongly divergent power series and large-order perturbation theory have become very popular since the pioneering works of Bender and Wu[1] and Simon[2] on the quantum anharmonic oscillator. Excellent reviews on this subject are available.[3,4]

The purpose of this paper is to show a new method for summing divergent power expansions that is very simple and requires no knowledge of the asymptotic behavior of the Taylor coefficients. The procedure is developed in Sec. II and consists of transforming the power series into a convergent succession by means of an order-dependent mapping obtained from a simple scaling relation. It is then applied to three well-known strongly divergent power series that are accurately summed in the most unfavorable strong-coupling limit.

In Sec. III we deal with a one-dimensional integral that may be considered to be either the classical partition function of the anharmonic oscillator or a zero-dimensional analog of some functional integrals encountered in ϕ^4-scalar field theory.[5] We consider the power series expansion for the lowest eigenvalue of the anharmonic oscillator in Sec. IV and that for the ground state of the linear confining potential model in Sec. V. Finally, further remarks on the method are made in Sec. VI.

II. THE METHOD

Motivated by a sort of semiclassical approach to parameter-dependent systems,[6,7] we have recently developed a new procedure (called functional method) that has proved to be successful in obtaining accurate results from strongly divergent power series by using a few perturbation terms.[8–10] Several models were treated; among them we can mention those studies in the present paper,[8–10] the Stark[10] and Zeeman[8,9] effects in hydrogen. Though acceptable results were obtained in all cases, the rearranged series included no more than ten perturbation terms so that it was not clearly proved whether they were convergent or merely asymptotic.

In this section we show an improved version of the above mentioned method that can be easily applied to a large number of problems in quantum and field theory. The viewpoint of the present approach is quite different from the previous one.[8–10]

Let $E(Z,\lambda)$ $(0<Z,\lambda<\infty)$ be a real, unknown function that obeys the asymptotic expansion

$$E(1,\lambda)=\sum_{i=0}^{\infty}E_i\lambda^i, \tag{1}$$

and the scaling relation

$$E(Z,\lambda)=Z^aE(1,\lambda Z^b), \tag{2}$$

where a and b are real numbers and $b<0$. It is our purpose to show how to obtain an accurate enough approximation to $E(1,\lambda)$ [and also to $E(Z,\lambda)$ in virtue of Eq. (2)] when the first $N+1$ coefficients E_i are available. This problem is interesting because it is often encountered in quantum and field theory as will be seen later on.

Our procedure is based upon the fact that, due to Eq. (2), the function

$$\bar{E}(K,\beta)=E(K\{1-\beta\},\beta), \tag{3}$$

where K and β are real, positive numbers, can be written as

$$E(1,\lambda)=K^{-a}(1-\beta)^{-a}\bar{E}(K,\beta), \tag{4}$$

where

$$\lambda=K^b\beta(1-\beta)^b. \tag{5}$$

Since $b<0$, this last equation maps $0\le\lambda<\infty$ onto $0\le\beta<1$.

To find an appropriate expansion for $E(1,\lambda)$ in powers of the bounded variable β we write

$$\bar{E}(K,\beta)=\sum_{i=0}^{\infty}\bar{E}_i(K)\beta^i. \tag{6}$$

In order to obtain the coefficients $\bar{E}_i(K)$ we rewrite (4) as $\bar{E}(K,\beta)=K^a(1-\beta)^aE(1,\lambda(\beta))$ and expand its right-hand side in powers of β by using the mapping (5) and the expansion (1). The result is

$$\bar{E}_j(K)=\sum_{i=0}^{j}(-1)^{j-i}\binom{a+bi}{j-i}K^{a+bi}E_i, \tag{7}$$

where $\binom{c}{i}=c(c-1)(c-2)\cdots(c-i+1)/i!$ and $\binom{c}{0}=1$.

According to Eq. (4), the sequence

$$SE_N(K,\beta)=K^{-a}(1-\beta)^{-a}S_N(K,\beta),$$

$$S_N(K,\beta)=\sum_{i=0}^{N}\bar{E}_i(K)\beta^i,\quad N=1,2,... \tag{8}$$

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will converge towards $E(1,\lambda)$ if $S_N(K,\beta)(N=1,2...)$ converges to $\bar{E}(K,\beta)$. A sufficient condition for this is that $S_N(K,1)$ converges to $\bar{E}(K,1)$ because $|\beta|<1$.

The parameter K plays a key role in obtaining a convergent succession and its proper value must be determined carefully. To this end notice that $\bar{E}(K,1)=E(0,1)$ is K independent. Therefore, if $S_N(K,1)$ converges towards $E(0,1)$, the curve $S_N(K,1)$ vs K will exhibit a plateau whose extension will increase as N increases. The existence of such a plateau is a suitable convergence criterion and it seems to be most reasonable to choose a K value that belongs to its flattest part. In this paper we use either the stationary point $K_N^S,(\partial S_N/\partial K)(K=K_N^S,\beta=1)=0$, with the smallest absolute value of the second derivative or the inflection point $K_N^I,(\partial^2 S_N/\partial K^2)(K=K_N^I,\beta=1)=0$, with the smallest absolute value of the first derivative. This point will be discussed in deeper detail in the next sections.

It follows from the discussion above that K [and thereby the mapping (5)] is order dependent. In this way, the original power series (1) has been transformed into the sequence (8) (with $K=K_N$).

On the other hand, the scaling relation (2) implies that

$$E(1,\lambda)=\lambda^{-a/b}E(\lambda^{1/b},1), \tag{9}$$

from which it follows that

$$\lim_{\lambda\to\infty}\lambda^{a/b}E(1,\lambda)=E(0,1), \tag{10}$$

provided $E(Z\to 0,1)$ exists. If in addition to this $E(Z,1)$ satisfies a Taylor expansion about $Z=0$ with coefficients e_i, we can write, according to Eq. (9), $E(1,\lambda)$ as

$$E(1,\lambda)=\lambda^{-a/b}\sum_{i=0}^{\infty}e_i\lambda^{i/b},\quad e_0=E(0,1), \tag{11}$$

which is valid for large enough λ values. Actually, each term SE_N of the sequence (8) obeys both λ- and $\lambda^{1/b}$-power series.

The existence of a scaling relation like (2) is not necessary for our method to apply. It often happens that the function we are interested in obeys two asymptotic expansions like those in Eqs. (1) and (11) which clearly determine the parameters a and b required for constructing the sequence SE_N.

There are two very interesting properties of our sequence SE_N that were pointed out in our earlier works on the functional method[8–10] and that can be easily proved using the present formulation. They are discussed in the following theorem.

Theorem:

(a) The stationary points $\bar{K}_N^S,(\partial SE_N/\partial K)_\lambda(K=\bar{K}_N^S)=0$, are independent of λ and thereby coincide with K_N^S.

(b) The inflection points $\bar{K}_N^I,(\partial^2 SE_N/\partial K^2)_\lambda(K=\bar{K}_N^I)=0$, are bounded functions of λ.

Proof: The first statement follows from the fact that

$$\left(\frac{\partial SE_N}{\partial K}\right)_\lambda=K^{-1}(1-\beta)^{-a}\{(b^{-1}+1)\beta-b^{-1}\}^{-1}\times\sum_{i=0}^{N+1}P_i(K)\beta^i, \tag{12}$$

where

$$P_i(K)=iJ_i-b^{-1}K\left(\frac{\partial J_i}{\partial K}\right)-(-a+i-1)J_{i-1}+K(b^{-1}+1)\left(\frac{\partial J_{i-1}}{\partial K}\right), \tag{13}$$

$J_i=K^{a/b}\bar{E}_i(k)$ if $0\le i\le N$ and $J_i=0$ otherwise. A straightforward manipulation of Eq. (7) shows that $P_i=0$ if $i<N+1$ which proves (a) because the stationary points $\bar{K}_N^S$ are the roots of $P_{N+1}(K)$.

Calculation of $(\partial^2 SE_N/\partial K^2)_\lambda$ shows that (b) is also true.

At present we do not know what general conditions are required for the sequence SE_N $(N=1,2,...)$ to converge towards the function $E(1,\lambda)$. However, in the next sections we will show that our method applies successfully to some well-known strongly divergent power series.

III. A SIMPLE ONE-DIMENSIONAL INTEGRAL

Our first example is the integral

$$E(Z,\lambda)=\pi^{-1/2}\int_0^\infty\exp(-Zx^2-\lambda x^4)dx, \tag{14}$$

that is often encountered in statistical mechanics[11] and field theory.[4,5]. It has also proved to be useful in studying large-order perturbation theory[4,5] because $E(Z,\lambda)$ leads to strongly divergent power series like (1) with coefficients

$$E_i=(-1)^i(4i)!/i!(2i)!2^{4i}. \tag{15}$$

Since $E(Z,\lambda)$ obeys (2) with $a=-1/2$ and $b=-2$, the method of Sec. II applies giving rise to the mapping

$$\lambda=K^{-2}\beta(1-\beta)^{-2} \tag{16}$$

that agrees with the one used by Seznec and Zinn-Justin.[5] From their results (obtained by the saddle-point approximation[5]) we know that the sequence SE_N converges for all λ values when $K^2=\text{const}+1.325\,487N$. Moreover, their numerical calculation shows that SE_N actually tends to $E(1,\lambda)$ as $N\to\infty$ (see Ref. 5).

In spite of the fact that our mapping equals that of Seznec and Zinn-Justin,[5] we determine K in a different way. However, it will be shown below that both methods yield identical results in the present case.

We have calculated all the stationary (K_N^S) and inflection (K_N^I) points of $S_N(K,1)$ for $1\le N\le 24$. There are one stationary and one inflection point when N is odd and two inflection points when N is even. A least-squares fitting of the last six points in each case yields

$$(K_N^S)^2=(1.169\pm 0.001)+(1.3253\pm 0.0003)N,\quad \text{odd } N, \tag{17}$$

and

$$(K_N^I)^2=(1.958\pm 0.008)+(1.323\pm 0.002)N,\quad \text{even } N. \tag{18}$$

To obtain Eq. (18) we have used the smaller K_N^I for each even N that corresponds to the smaller value of $|(\partial S_N/\partial K)(K=K_N^I)|$. Both results are in excellent agreement with those of Seznec and Zinn-Justin[5] who choose K_N so that $\bar{E}_N$ vanishes.

When determining K_N by either (17) or (18), our succession $S_N(K_N,1)$ converges towards $E(0,1)$ from below yielding

$$S_N(K_N,1)=1.022\,765\,669, \tag{19}$$

when $N=23$ (K_N^S) or $N=24$ (K_N^I), respectively. The agreement with the exact result

$$E(0,1)=\Gamma(\tfrac{1}{4})/2\pi^{1/2}=1.022\,765\,672... \tag{20}$$

is excellent. Since $E(0,1)$ corresponds to the limit $\lambda\to\infty$ [cf. Eq. (10)], we are sure that even more accurate results will be obtained for all finite λ values.

The remaining inflection points that appear for all N values can be accurately fitted by the straight line (using the last 12 points)

$$K_N^I=(0.912\pm0.003)+(1.1534\pm0.0007)N. \tag{21}$$

It determines a sequence $S_N(K_N,1)$ that converges to a wrong limit ($=0.9203...$). Straight lines K_N vs N are always present in our method and they always give rise to sequences converging to wrong limits that were not predicted by Seznec and Zinn-Justin.[5] Fortunately, these spurious sequences are put aside by the requirement of smallest $|(\partial^2 S_N/\partial K^2)(K_N^S,1)|$ and $|(\partial S_N/\partial K)(K_N^I,1)|$. Moreover, it seems to be a general rule that the straight lines K^{-b} vs N give rise to correct sequences.

Most problems in quantum mechanics lead to more complicated patterns of stationary and inflection points than that just discussed above. However, our numerical investigation suggests that they all are quite similar, as will be shown later on in the next sections.

IV. THE ANHARMONIC OSCILLATOR

The anharmonic oscillator

$$H(Z,\lambda)=p^2+Zx^2+\lambda x^4,\quad p=-i\frac{d}{dx}, \tag{22}$$

is also useful in checking our method because the perturbation series for its eigenvalues are known to be strongly divergent and many Taylor coefficients have been calculated for the lowest eigenvalue.[1] Their asymptotic form is also well-known ($Z=1$)[1,2]:

$$E_n\approx-2(6/\pi^3)^{1/2}(-\tfrac{3}{2})^n(n-\tfrac{1}{2})!. \tag{23}$$

It immediately follows from the Symanzik's theorem[2] that any eigenvalue $E(Z,\lambda)$ of $H(Z,\lambda)$ obeys (2) with $a=\frac{1}{2}$ and $b=-\frac{3}{2}$. This leads us to one of the order-dependent mappings studied by Seznec and Zinn-Justin[5]:

$$\lambda=K^{-3/2}\beta(1-\beta)^{-3/2}. \tag{24}$$

It is worth noticing that $\bar{E}(K,\beta)$ [cf. Eq. (3)] is an eigenvalue of the Hamiltonian operator

$$H(K\{1-\beta\},\beta)=p^2+Kx^2+\beta(x^4-Kx^2). \tag{25}$$

It is not difficult to prove that in this particular case our method is exactly equivalent to Caswell's generalized Wick ordering[12] provided K is properly chosen. However, the former is more general than the latter that only applies to anharmonic oscillators and double-well potentials.[12] An example of this last sort of model is obtained in our case when $\beta>1$ because the Hamiltonian operator (25) obeys $H(K\{1-\beta\},\beta)=K^{1/2}(\beta-1)^{1/2}$ $\times H(-1,\beta K^{-3/2}(\beta-1)^{-3/2})$. We therefore define

$$\lambda=K^{-3/2}\beta(\beta-1)^{-3/2}. \tag{26}$$

Unfortunately, Eq. (26) maps $0\le\lambda<\infty$ into $\infty>\beta>1$ due to which we cannot obtain accurate eigenvalues for arbitrarily small λ values.[12] This is reasonable because we have two infinitely deep wells when $\lambda\to0$.

In what follows we show the results obtained for the lowest eigenvalue of (22) (with $Z=1$) using the perturbation coefficients given in Ref. 1. We begin with an analysis of the distribution of the stationary and inflection points of $S_N(K,1)$ in the $K^{3/2}$-N plane. Since both sets of points give rise to similar patterns, only the inflection points will be discussed here in detail. These are shown in Fig. 1. Each of the full lines A–D, which are straight lines K vs N, generates a spurious sequence that converges to a wrong limit. Though their convergence is quite slow and we cannot handle enough perturbation coefficients to obtain their limits accurately, we can estimate them to be about of 1.3, 1.060 34, 1.060 3622, 1.060 362 09, respectively. Obviously, as we pass from A to D we approach the exact result[13]

$$E(0,1)=1.060\,362\,090\,5... \tag{27}$$

more and more closely. This step-by-step approximation to the eigenvalue was previously pointed out by Caswell.[12] The path E that appears in Fig. 1 is not reasonable because it means a decreasing order dependence. Therefore, it must be avoided.

As argued before, the proper sequence is obtained by keeping, for each N value, the inflection point with the smallest absolute value of the first derivative. It corresponds to retain the smallest K_N^I for each N. With such a sequence we obtain

$$E(0,1)^{\text{present}}=1.060\,362\,09\pm10^{-8}, \tag{28}$$

that agrees very closely with (27). A similar analysis of the stationary points yields exactly the same result. Clearly, our method enables us to obtain the eigenvalues of the quartic oscillator [$H(0,1)=p^2+x^4$] by applying perturbation theory to the anharmonic oscillator (22).

Since $\beta=1$ ($\lambda\to\infty$ or $Z=0$) is the most unfavorable case, we expect our sequence SE_N will approach an eigenvalue of $H(1,\lambda)$ very closely for all λ values. In Table I we compare our results with Banerjee's very accurate nonperturbative calculation[14] showing an excellent agreement when using either the inflection or stationary points. The accuracy of our results is almost independent of λ.

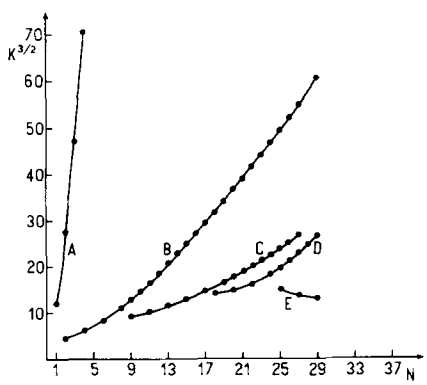

FIG. 1. Inflection points of $S_N(K,1)$ for the lowest eigenvalue of the anharmonic oscillator $H(1,\lambda)=p^2+x^2+\lambda x^4$.

TABLE I. Lowest eigenvalue of the anharmonic oscillator $H(1,\lambda)=p^2+x^2+\lambda x^4$.

λ	$E(1,\lambda)^a$	$E(1,\lambda)^b$	error %	$E(1,\lambda)^c$	error %
10^{-3}	1.000 748 692 67	1.000 748 692 9	2.0×10^{-8}	1.000 748 692 4	3.0×10^{-8}
1	1.392 351 641 53	1.392 351 641 0	3.6×10^{-8}	1.392 351 641 3	1.4×10^{-8}
10^4	22.861 608 870 27	22.861 608 82	2.2×10^{-7}	22.861 608 700	7.4×10^{-7}

[a] "exact" (see Ref. 14).
[b] Equation (8) with $N=24$ and $K^I_{24}=6.916\,413\,786$.
[c] Equation (8) with $N=23$ and $K^S_{23}=6.167\,663\,727$.

V. THE LINEAR CONFINING POTENTIAL

The Hamiltonian operator

$$H(Z,\lambda)=p^2/2-Z/r+\lambda r,\quad p=-i\nabla, \tag{29}$$

proves to be very useful in particle physics (see Ref. 15 and references therein). It has also received considerable attention[16–19] because its eigenvalues lead to strongly divergent perturbation series. In particular, the asymptotic form of the perturbation coefficients for the lowest eigenvalue of $H(1,\lambda)$ is known to be[19]

$$E_n\approx-(18/\pi e^3)(-3/2)^n n(n!). \tag{30}$$

Clearly, this series diverges more strongly (and therefore it is more difficult to sum) than that for the anharmonic oscillator [cf. Eq. (21)].

A simple scaling argument shows that our method applies to this case with $a=2$ and $b=-3$ yielding

$$E(1,\lambda)=K^{-2}(1-\beta)^{-2}JE(K,\beta),$$
$$\lambda=K^{-3}\beta(1-\beta)^{-3}. \tag{31}$$

It is worth noticing that $\bar{E}(K,\beta)$ is an eigenvalue of

$$H(K\{1-\beta\},\beta)=p^2/2-K/r+\beta(\lambda r+K/r) \tag{32}$$

that equals the partition of the Hamiltonian operator proposed by Killingbeck[16] and Austin and Killingbeck.[17] However, they did not take advantage of the scaling relation (31) and their power series rearranged as Padé approximants proved to converge very slowly.[17] Owing to this, their results are of acceptable accuracy only for λ values smaller than 1.0 (see Refs. 16 and 17). We will show below that our method yields accurate results even for λ values as large as $\lambda=500$. To this end we make use of the perturbation coefficients obtained by Privman.[20]

One of the most attractive features of our method is that the patterns of stationary and inflection points for all models studied are quite similar. It seems to be a general rule that the stronger the divergence of the perturbation series the larger the number of points K_N in the same region of the K^{-b}-N plane. This fact is illustrated in Fig. 2 where we show the stationary points of $S_N(K,1)$ for the lowest eigenvalue of (29) (with $Z=1$). The full lines labeled A–E in Fig. 2 are straight lines K_N vs N that give rise to spurious sequences converging to wrong limits. However, the convergence in this case is so slow that we need a much larger number of perturbation terms in order to have acceptable estimates of these limits. Also in this case, we see a line (F) with a negative slope. A more careful calculation, using more perturbation terms, is required to show whether such negative order dependences are due to numerical errors.

The sequence $S_N(K_N,1)$ (chosen as discussed in Secs. III and IV) converges too slowly in this case to obtain a close approach to $E(0,1)=1.8557\ldots$. This is due to the fact that the present perturbation series diverges more strongly than those studied previously. Our best estimate is $E(0,1)^{\text{present}}=1.85\pm0.02$.

The present perturbation calculation of $E(1,\lambda)$ is accurate enough for most purposes. Table II shows that our results agree closely with those obtained by numerical integration of the Schrödinger equation[21] in quite a wide range of λ values. As far as we know, there is no other perturbation calculation reported in the literature that yields such accurate results with only 13 perturbation coefficients. For example, our estimate of $E(1,\lambda)$ is somewhat less accurate in the small- and intermediate-λ regime than that obtained by a (16/15) Borel–Padé approximant[18] that requires 31st-order perturbation theory but is a much better approach to the "exact" eigenvalue[21] in the strong-coupling regime. This is due to the fact that $|\lambda^{-2/3}(16/15)|$ tends to infinity as $\lambda\to\infty$ instead of being an approximation to $E(0,1)$.

VI. FURTHER COMMENTS

The method developed in this paper is very simple, requires little computational effort, and applies to a large variety of problems in quantum and field theory. Two good examples of the former are the Zeeman[22] and Stark[23] effects in hydrogen. These models, which have received considerable attention owing to their many physical applications (see Refs. 22 and 23 and references therein), lead to strongly divergent perturbation series[24,25] and their Hamiltonian operators obey scaling relations like (2).

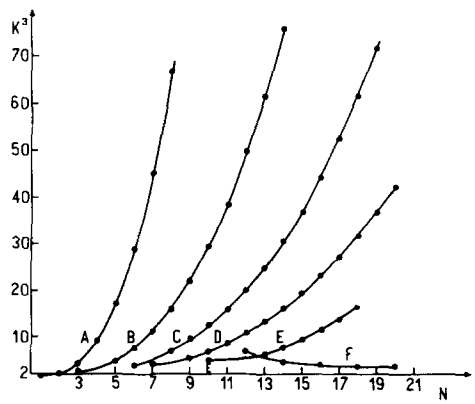

FIG. 2. Stationary points of $S_N(K,1)$ for the lowest eigenvalue of $H(1,\lambda)=p^2/2-1/r+\lambda r$.

TABLE II. Lowest eigenvalue of $H(1,\lambda) = p^2/2 - 1r + \lambda r$.

λ	$E(1,\lambda)^a$	$E(1,\lambda)^b$	error %
0.685 871 06	0.284 113 4	0.284 115	5.6×10^{-4}
4	2.796 002 8	2.795 754	8.9×10^{-3}
500	108.466 431	108.365 80	9.3×10^{-2}

[a] Equation with $N = 13$ and $K^S_{13} = 1.830\ 718\ 5377$.
[b] "exact" (see Ref. 21).

Our method proves to be successful also in calculating the rotational energy of diatomic and symmetric-top molecules in electric and magnetic fields.[26] In such cases there is no scaling relation and the parameters a and b are obtained from asymptotic expansions like (11) (see Ref. 26).

Some interesting features of our method that were pointed out before require further study. It would be useful to prove why one obtains similar patterns of stationary and inflection points in the K^{-b}-N plane for all problems having bound states. It would be particularly fruitful to know the reasons for the occurrence of spurious sequences based upon straight lines K_N vs N. All these points are being studied at present in our laboratory and conclusions will appear elsewhere in a forthcoming paper.

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Bound state energy eigenvalues for a general class of one-dimensional problems on the whole axis $(-\infty, \infty)$ via the Prüfer transformation

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(Received 30 November 1983; accepted for publication 11 May 1984)

An extension of the Prüfer phase function method for the bound state energy calculation is presented. It is applicable to one-dimensional problems described by the Schrödinger equation on the whole axis $(-\infty,\infty)$ with a general class of potentials. Theorems are given which are a generalization of the analogous ones concerning the half-axis $(0,\infty)$ problems that have been presented in previous papers. The method is suitable especially for numerical calculations of the bound state energy eignevalues.

PACS numbers: 03.65.Ge

I. INTRODUCTION

In a number of fields in physics the bound state energies (BSE) of a system described by the one-dimensional Schrödinger equation (SE) with a real potential are of interest.[1] Mostly, for the potential of a general form, the BSE have to be calculated numerically.

In a previous paper,[2] the problem of the BSE for a system described by the three-dimensional SE with a real central potential was investigated in terms of the (modified) Prüfer transformation (PT)[3] and the theoretical framework of a method for the numerical calculation of the BSE was established. The method utilizes the PT and enables one to find the BSE with a known accuracy using only the values of a phase function at some distant but finite point.

The aim of the present paper is to modify the method treated in Ref. 2, which, in fact, applies to a problem formulated on the half-axis $(0,\infty)$, so as to make it applicable to a one-dimensional problem formulated on the whole axis $(-\infty,\infty)$.

We consider the SE,

$$\left\{\frac{d^2}{dx^2}+\epsilon-w(x)\right\}\psi(x,\epsilon)=0, \tag{1.1}$$

for $x\in(-\infty,\infty)$, where ϵ is a real parameter (energy) and the function (potential) $w(x)$ has the following properties: (i) $w(x)$ is a real function, finite for $x\in(-\infty,\infty)$ and continuous except for a finite number of points; (ii) there exist limits $\lim_{x\to+\infty} w(x)=w(+\infty)$, $\lim_{x\to-\infty} w(x)=w(-\infty)$ and it holds $\min\{w(+\infty),\ w(-\infty)\} > -\infty$ while it can be $\max\{w(+\infty), w(-\infty)\}=+\infty$.

Denote $\tilde{w}=\min\{w(+\infty), w(-\infty)\}$. In the following, only the values of $\epsilon\in(-\infty,\tilde{w})$ and only the potential functions satisfying (i) and (ii) are considered. We shall refer to them as to the ϵ, $w(x)$ with the properties P.

It is known[4] that there exists a self-adjoint operator L which is the (unique) extension of the operator L_0 induced by the differential expression $\{-d^2/dx^2+w(x)\}$ with $w(x)$ satisfying (i) and (ii) on the class of functions $C_0^\infty(R)$. The BSE we are interested in are the eigenvalues of the operator L contained in the interval $(-\infty,\tilde{w})$. According to the asymptotic behavior of solutions of Eq. (1.1) with $w(x)$, ϵ having the properties P[2,5] the BSE problem can be formulated in the following way.

Let $\psi(x,\epsilon)$ be a solution of Eq. (1.1) with $w(x)$, ϵ having the properties P. Then the BSE problem is defined by

$$\psi(-\infty,\epsilon)=0, \tag{1.2a}$$

$$\psi(+\infty,\epsilon)=0, \tag{1.2b}$$

and $\psi(x,\epsilon)$ should be a continuous function of x together with its first derivative.

It is convenient to treat individually the cases of a symmetric potential $w(x)=w(-x)$, $x\in(-\infty,\infty)$ and of a general one. It is known that in the former case the solutions of Eq. (1.1) satisfying (1.2) are either even or odd functions of x. Denote these solutions $\psi_A(x,\epsilon)$, $\psi_B(x,\epsilon)$, respectively. Then,

$$\psi_A'(0,\epsilon)=0,$$

$$\psi_B(0,\epsilon)=0,$$

where the prime denotes the derivative by x. Each of these conditions defines a solution of Eq. (1.1) which is unique up to a multiplicative constant. We take the choice

$$\psi_A(0,\epsilon)=1,\quad \psi_A'(0,\epsilon)=0, \tag{1.3a}$$

$$\psi_B(0,\epsilon)=0,\quad \psi_B'(0,\epsilon)=1. \tag{1.3b}$$

The conditions (1.3) are crucial for the unique definition of phase functions by means of which the BSE can be determined. If the potential is not a symmetric function one has to utilize the asymptotic behavior of a function $v(x,\epsilon)$ defined by the relation

$$v(x,\epsilon)=\psi(x,\epsilon)/\psi'(x,\epsilon) \tag{1.4}$$

to get a condition of the same meaning as (1.3). In (1.4) the function $\psi(x,\epsilon)$ is a solution of Eq. (1.1) with a nonsymmetric potential $w(x)$ and with ϵ having the properties P. If this $\psi(x,\epsilon)$ satisfies (1.2a) the following statements are valid:

$$\lim_{x\to-\infty} v(x,\epsilon)=(w(-\infty)-\epsilon)^{-1/2},\quad \text{if } w(-\infty)<+\infty, \tag{1.5a}$$

$$\lim_{x\to-\infty} v(x,\epsilon)=0,\quad \text{if } w(-\infty)=+\infty, \tag{1.5b}$$

there exists $x_0\in(-\infty,\infty)$ such that

$$v(x,\epsilon)>0,\quad \text{for } x\in(-\infty,x_0). \tag{1.5c}$$

The proof can be carried out in full analogy with that of Lemma 2.1 and Theorem 2.3 in Ref. 5.

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The conditions (1.5) define a solution of Eq. (1.1) up to a multiplicative constant. We choose the solution $\psi = \psi_C(x,\epsilon)$ of Eq. (1.1) satisfying the corresponding relation (1.5) and the condition

$$\int_{-\infty}^{0} \psi_C^2(x,\epsilon)dx = \frac{1}{2}. \tag{1.6}$$

The conditions (1.5) and (1.6) replace (1.3) when the potential has a general nonsymmetric form.

In the following we define the phase functions mentioned before by means of the PT. We give theorems which establish the connection between asymptotic properties of the phase functions and the BSE problem defined above. Since there are three different sets of conditions (1.3a), (1.3b), and (1.5), (1.6) which are essential for the definition of a phase function the three cases are treated individually, i.e., (A) a symmetric potential $w(x)$ and even bound state functions (BSF), (B) a symmetric potential $w(x)$ and odd BSF, (C) a general nonsymmetric potential $w(x)$.

In Sec. II we give the definitions of the proper phase functions in each of the above cases. In Sec. III the theorems essential for the BSE calculation by means of the phase functions are formulated. Section IV contains some concluding remarks.

II. TRANSFORMATION TO PHASE FUNCTIONS

(A) Let ϵ, $w(x)$ in Eq. (1.1) have the properties P, $w(x)$ being a symmetric function of x. Consider the solution $\psi_A(x,\epsilon)$ of Eq. (1.1) satisfying (1.3a) and perform the PT[6]

$$\begin{aligned} &\psi_A(x,\epsilon) = p_A(x,\epsilon)\cos z_A(x,\epsilon), \\ &\psi_A'(x,\epsilon) = -p_A(x,\epsilon)\sin z_A(x,\epsilon). \end{aligned} \tag{2.1}$$

Here $z_A(x,\epsilon)$ is the phase function mentioned before.

We require the new functions p_A, z_A to be continuous functions of x, $p_A(x,\epsilon) > 0$ for $x \in (-\infty,\infty)$ and according to (1.3a) we can choose

$$z_A(0,\epsilon) = 0. \tag{2.2}$$

These conditions define the $z_A(x,\epsilon)$, $p_A(x,\epsilon)$ in (2.1) uniquely. Equations (1.1) and (2.1) then imply

$$z_A' = \sin^2 z_A + (\epsilon - w(x))\cos^2 z_A. \tag{2.3}$$

On the other hand, the condition (2.2) defines uniquely one of the solutions of Eq. (2.3).[7] It is easy to show that there is a one-to-one correspondence between the solution $\psi_A(x,\epsilon)$ of Eq. (1.1) satisfying (1.3a) and the solution $z_A(x,\epsilon)$ of Eq. (2.3) satisfying (2.2) (cf. Ref. 8).

(B) Let ϵ, $w(x)$ in Eq. (1.1) have the properties P, $w(x)$ being a symmetric function of x. Consider the solution $\psi_B(x,\epsilon)$ of Eq. (1.1) satisfying (1.3b) and perform the PT

$$\begin{aligned} &\psi_B(x,\epsilon) = p_B(x,\epsilon)\sin z_B(x,\epsilon), \\ &\psi_B'(x,\epsilon) = p_B(x,\epsilon)\cos z_B(x,\epsilon). \end{aligned} \tag{2.4}$$

Again, $z_B(x,\epsilon)$ is the discussed phase function. We require p_B, z_B to be continuous functions of x, $p_B(x,\epsilon) > 0$ for $x \in (-\infty,\infty)$ and according to (1.3b) we can choose

$$z_B(0,\epsilon) = 0. \tag{2.5}$$

These conditions define the functions p_B, z_A in (2.4) uniquely.

It follows from Eqs. (1.1) and (2.4) that

$$z_B' = \cos^2 z_B + (\epsilon - w(x))\sin^2 z_B. \tag{2.6}$$

Again, there is just one solution $z_B(x,\epsilon)$ of Eq. (2.6) satisfying (2.5) and there is a one-to-one correspondence between this $z_B(x,\epsilon)$ and the solution $\psi_B(x,\epsilon)$ of Eq. (1.1) satisfying (1.3b).

(C) Let ϵ, $w(x)$ in Eq. (1.1) have the properties P, $w(x)$ being a nonsymmetric function of x. Consider the solution $\psi_C(x,\epsilon)$ of Eq. (1.1) satisfying (1.5) and (1.6) and perform the PT

$$\begin{aligned} &\psi_C(x,\epsilon) = p_C(x,\epsilon)\sin z_C(x,\epsilon), \\ &\psi_C'(x,\epsilon) = p_C(x,\epsilon)\cos z_C(x,\epsilon). \end{aligned} \tag{2.7}$$

Now, we have to find conditions defining the functions p_C, z_C in (2.7) uniquely. Again, we require $p_C(x,\epsilon) > 0$ for $x \in (-\infty,\infty)$ and that both functions p_C, z_C be continuous functions of x. It follows from Eq. (2.7) that

$$\tan z_C(x,\epsilon) = v_C(x,\epsilon), \tag{2.8}$$

where $v_C(x,\epsilon)$ is defined by Eq. (1.4) with $\psi = \psi_C$. According to the conditions (1.5a) and (1.5b)

$$\lim_{x\to-\infty} \tan z_C(x,\epsilon) = \begin{cases} (w(-\infty)-\epsilon)^{-1/2}, & \text{if } w(-\infty) < \infty, \\ 0, & \text{if } w(-\infty) = \infty, \end{cases} \tag{2.9a}$$

and there exists $x_0 \in (-\infty,\infty)$ such that

$$\tan z_C(x,\epsilon) > 0, \quad \text{if } x \in (-\infty, x_0). \tag{2.9b}$$

Denote $\lim_{x\to-\infty} z_C(x,\epsilon) = z_C(-\infty,\epsilon)$ and choose $z_C(x,\epsilon)$ so as

$$z_C(-\infty,\epsilon) = \begin{cases} \arctan (w(-\infty)-\epsilon)^{-1/2}, & \text{if } w(-\infty) < \infty, \\ 0, & \text{if } w(-\infty) = \infty. \end{cases} \tag{2.10}$$

Equations (2.7) and (2.10) together with the requirement $p_C > 0$ define uniquely $p_C = p_C(x,\epsilon)$, $z_C = z_C(x,\epsilon)$ as continuous functions of x. It follows from Eqs. (1.1) and (2.7) that

$$z_C' = \cos^2 z_C + (\epsilon - w(x))\sin^2 z_C. \tag{2.11}$$

It can be proved that there is just one solution $z_C(x,\epsilon)$ of Eq. (2.11) satisfying (2.9b) and (2.10) and there can be established a one-to-one correspondence between this function $z_C(x,\epsilon)$ and the solution $\psi_C(x,\epsilon)$ of Eq. (1.1) satisfying (1.5) and (1.6). The exact proof of this statement is based on a reconstruction of functions $\psi_C(x,\epsilon)$, $\psi_C'(x,\epsilon)$ by means of the $z_C(x,\epsilon)$ satisfying (2.9b), (2.10), and (2.11) (for details see Ref. 8) and on the asymptotic behavior of solutions of Eq. (1.1) with the considered $w(x)$, ϵ.[5]

III. PHASE FUNCTIONS AND THE BSE PROBLEM

The phase functions z_A, z_B, z_C defined in the previous section have a number of interesting properties. For instance, $z_C(x,\epsilon)$ is a montonically increasing function of the parameter $\epsilon \in (-\infty, \tilde{w})$ for any fixed $x \in (-\infty,\infty)$ and the

same is valid for $z_A(x,\epsilon)$, $z_B(x,\epsilon)$ if the chosen fixed x is positive. The proof can be carried out in analogy with that of Lemma A3 in Ref. 2. Further, the z_A, z_B, z_C are continuous functions of the parameter $\epsilon\in(-\infty,\tilde{w})$ for any fixed $x\in(-\infty,\infty)$. For z_A, z_B it follows from standard theorems about continuity of solutions of a differential equation with respect to the parameter.[7] In the case of z_C it can be proved employing a procedure analogous to those used in Appendix A in Ref. 2.

In this section we formulate two theorems which establish the connection between asymptotic properties of the functions z_A, z_B, z_C and the BSE problem. It is understood that z_A, z_B, z_C correspond to the aforementioned cases A, B, C, respectively.

Theorem 1: Let the parameter ϵ and the potential $w(x)$ in Eq. (1.1) have the properties P. Denote $z_{A(B,C)}(\infty,\epsilon) = \lim_{x\to+\infty} z_{A(B,C)}(x,\epsilon)$. Then (1) $z_{A(B,C)}(\infty,\epsilon)$ is piecewise continuous and nondecreasing and it holds

(A) $z_A(\infty,\epsilon)\geqslant -\pi/2$,

(B),(C) $z_{B(C)}(\infty,\epsilon)\geqslant 0$.

(2) ϵ is a discontinuity point of $z_{A(B,C)}(\infty,\epsilon)$ iff ϵ is a BSE; then

$$\lim_{\eta\to 0^+}\{z_{A(B,C)}(\infty,\epsilon+\eta) - z_{A(B,C)}(\infty,\epsilon-\eta)\} = \pi.$$

(3) Choose some $\epsilon_0\in(-\infty,\tilde{w})$. There exists an integer $k\geqslant 0$ such that

(A) $-\pi/2 + k\pi \leqslant z_A(\infty,\epsilon_0) < \pi/2 + k\pi$,

(B),(C) $k\pi \leqslant z_{B(C)}(\infty,\epsilon_0) < (k+1)\pi$.

Then (A) there are just k BSE less than or equal to ϵ_0 corresponding to even BSF, (B) there are just k BSE less than or equal to ϵ_0 corresponding to odd BSF, (C) there are just k BSE less than or equal to ϵ_0. ■

Thus, were the functions $z_A(\infty,\epsilon)$ and $z_B(\infty,\epsilon)$, respectively, the function $z_C(\infty,\epsilon)$, reconstructed in the interval $(-\infty,\tilde{w})$ and their discontinuities found, all the BSE less than $\tilde{w}$ would be determined. However, mostly we are not able to find the functions z_A, z_B, z_C analytically and in numerical calculations we are not able to reconstruct $z_{A(B,C)}(\infty,\epsilon)$ exactly. The point is that the properties of $z_{A(B,C)}(\infty,\epsilon)$ are signalled by the behavior of $z_{A(B,C)}(x_0,\epsilon)$ with a sufficiently large but finite x_0.

Theorem 2: Let $w(x)$, ϵ_0 in Eq. (1.1) have the properties P, and $\tilde{x}\in(0,\infty)$ be such that $w(x) - \epsilon_0 > 0$ for $x\in\langle\tilde{x},\infty)$. Choose some $x_0\in(\tilde{x},\infty)$. Then the following statements are valid.

(1) If

(A) $-\pi/2 + n\pi \leqslant z_A(x_0,\epsilon_0) \leqslant n\pi$,

(B),(C) $n\pi \leqslant z_{B(C)}(x_0,\epsilon_0) \leqslant (n+\frac{1}{2})\pi$

for some integer $n\geqslant 0$, then (A) there are just n BSE in the interval $(-\infty,\epsilon_0)$ belonging to even BSF, (B) there are just n BSE in $(-\infty,\epsilon_0)$ belonging to odd BSF, (C) there are just n BSE in $(-\infty,\epsilon_0)$.

(2) If

(A) $n\pi < z_A(x_0,\epsilon_0) < (n+\frac{1}{2})\pi$,

(B), (C) $(n+\frac{1}{2})\pi < z_{B(C)}(x_0,\epsilon_0) < (n+1)\pi$

for some integer $n\geqslant 0$, then the same statements as in (1) are valid with "n BSE" replaced by "n or (n + 1) BSE."

(3) The BSE ϵ_n, $n = 1,2,\ldots$, is localized within an interval $I_{n,x_0} = (\bar{\epsilon}_{n,x_0}, \bar{\bar{\epsilon}}_{n,x_0})$, where

(A) $z_A(x_0, \bar{\epsilon}_{n,x_0}) = (n-1)\pi$,

$z_A(x_0, \bar{\bar{\epsilon}}_{n,x_0}) = (n-\frac{1}{2})\pi$,

(B),(C) $z_{B(C)}(x_0, \bar{\epsilon}_{n,x_0}) = (n-\frac{1}{2})\pi$,

$z_{B(C)}(x_0, \bar{\bar{\epsilon}}_{n,x_0}) = n\pi$.

(4) The length of any interval I_{n,x_0}, $n = 1,2,\ldots$, decreases montonically to zero when $x_0\to\infty$. ■

The proofs of both theorems can be carried out in analogy with those of Lemma 2.7 and Theorem 3.1 in Ref. 2.

IV. SUMMARY AND CONCLUDING REMARKS

(1) The conclusions resulting from Theorem 2 are quite analogous to those obtained in Ref. 2: Taking x_0 sufficiently large and investigating the function $z_{A(B,C)}(x_0,\epsilon)$ in the interval $(-\infty,\epsilon_0)$ intervals can be found, any of which contains just one BSE [corresponding to the BSF of the certain parity in the cases (A), (B)] smaller than ϵ_0. Increasing x_0 one can make the length of these "BSE intervals" small enough to obtain the BSE with a desired accuracy.

(2) The phase function z_C discussed in the case of a general nonsymmetric potential is defined by the boundary condition (2.10) at the point $x = -\infty$. In practical calculations one starts with the integration of Eq. (2.11) at some distant but finite point $x_0 < 0$. To do this one has to find the analytic asymptotic form of $z_C(x,\epsilon)$ for $x\to-\infty$. It can be obtained by the help of standard theorems about the asymptotic behavior of solutions of Eq. (1.1)[9] and using Eq. (2.8). The starting point x_0 and the starting value $z_C(x_0,\epsilon)$ for the integration should be then chosen according to the asymptotic formulas and the intervals of their validity.

(3) To be sure that using the function z_C determined by an asymptotic starting value one obtains the correct BSE intervals, one needs the corresponding solutions of Eq. (2.11) to be stable. Our numerical calculations show a high stability of these solutions. Theoretical aspects of this problem are under investigation.

(4) In the case of a symmetric potential one can choose either the method using the functions z_A, z_B or that one employing the function z_C. Both methods are of the same efficiency but using the former one need not carry out asymptotic estimates.

ACKNOWLEDGMENTS

The authors are indebted to M. Havlíček for numerous valuable discussions and to J. Blank for a critical reading of the manuscript.

APPENDIX A: NUMERICAL RESULTS

To illustrate the efficiency of the presented method for the BSE calculation we give some numerical results obtained with it in Tables I and II.

Table I contains lower and upper bounds on BSE for the potential $w(x)$

TABLE I. The bounds on the BSE for the potential $w(x) = V_0$, if $x \in (-\infty, 0\rangle$ and $w(x) = -0.1/(x - x_0)$, if $x \in (0, \infty)$. For simplicity we write, e.g., $0.644\,246\binom{4}{8}$ instead of $^{0.644\,2464}_{0.644\,2468}$.

	$V_0 = 100.$ $x_0 = -1.$	$V_0 = 0.5.$ $x_0 = -1.$	$V_0 = 100.$ $x_0 = -50.$
$-\epsilon_1$	$^{0.218\,0230}_{0.218\,0230} \cdot 10^{-2}$	$^{0.265\,7386}_{0.265\,7388} \cdot 10^{-2}$	$^{0.549\,2423}_{0.549\,2427} \cdot 10^{-3}$
$-\epsilon_2$	$0.582\,8286 \cdot 10^{-3}$	$0.644\,246\binom{4}{8} \cdot 10^{-3}$	$0.248\,918\binom{2}{4} \cdot 10^{-3}$
$-\epsilon_3$	$0.265\,0564 \cdot 10^{-3}$	$0.283\,438\binom{1}{2} \cdot 10^{-3}$	$0.142\,9734 \cdot 10^{-3}$
$-\epsilon_4$	$0.150\,8348 \cdot 10^{-3}$	$0.158\,629\binom{0}{2} \cdot 10^{-3}$	$0.929\,031\binom{1}{9} \cdot 10^{-4}$
$-\epsilon_5$	$0.972\,12\binom{49}{50} \cdot 10^{-4}$	$0.101\,215\binom{3}{4} \cdot 10^{-3}$	$0.652\,321\binom{3}{7} \cdot 10^{-4}$
$-\epsilon_6$	$0.678\,255\binom{0}{4} \cdot 10^{-4}$	$0.701\,46\binom{69}{72} \cdot 10^{-4}$	$0.483\,237\binom{3}{6} \cdot 10^{-4}$
$-\epsilon_7$	$0.499\,98\binom{28}{32} \cdot 10^{-4}$	$0.514\,62\binom{16}{20} \cdot 10^{-4}$	$0.372\,351\binom{2}{5} \cdot 10^{-4}$
$-\epsilon_8$	$0.383\,764\binom{4}{7} \cdot 10^{-4}$	$0.393\,58\binom{18}{22} \cdot 10^{-4}$	$0.295\,699\binom{8}{9} \cdot 10^{-4}$
$-\epsilon_9$	$0.303\,816\binom{3}{5} \cdot 10^{-4}$	$0.310\,717\binom{5}{7} \cdot 10^{-4}$	$0.240\,50\binom{48}{50} \cdot 10^{-4}$
$-\epsilon_{10}$	$0.246\,478\binom{0}{1} \cdot 10^{-4}$	$0.251\,512\binom{3}{5} \cdot 10^{-4}$	$0.199\,442\binom{0}{1} \cdot 10^{-4}$
$-\epsilon_{11}$	$0.203\,962\binom{8}{9} \cdot 10^{-4}$	$0.207\,747\binom{3}{4} \cdot 10^{-4}$	
$-\epsilon_{12}$	$0.171\,569\binom{2}{4} \cdot 10^{-4}$	$0.174\,485\binom{6}{8} \cdot 10^{-4}$	
$-\epsilon_{13}$	$0.146\,32\binom{19}{20} \cdot 10^{-4}$	$0.148\,616\binom{6}{7} \cdot 10^{-4}$	
$-\epsilon_{14}$	$0.126\,263\binom{5}{6} \cdot 10^{-4}$		
$-\epsilon_{15}$	$0.110\,063\binom{8}{9} \cdot 10^{-4}$		
$-\epsilon_{16}$	$0.967\,9\binom{293}{301} \cdot 10^{-5}$		
$-\epsilon_{17}$	$0.857\,85\binom{12}{20} \cdot 10^{-5}$		
$-\epsilon_{18}$	$0.765\,53\binom{67}{74} \cdot 10^{-5}$		
$-\epsilon_{19}$	$0.687\,3\binom{596}{602} \cdot 10^{-5}$		
$-\epsilon_{20}$	$0.620\,57\binom{37}{41} \cdot 10^{-5}$		

$$w(x) = V_0, \quad \text{if } x \in (-\infty, 0\rangle,$$
$$w(x) = -0.1/(x - x_0), \quad \text{if } x \in (0, \infty), \tag{A1}$$

where $V_0 > 0$, $x_0 < 0$ are constants. Potentials of this form are interesting for solid state physics. The potential defined by (A1) belongs to the class (C) discussed in the present paper. We give the bounds on the BSE in the following three cases:

(1) $V_0 = 100, \quad x_0 = -1,$

(2) $V_0 = 0.5, \quad x_0 = -1,$

(3) $V_0 = 100, \quad x_0 = -50.$

As mentioned in Sec. I, the phase function method discussed in the present paper is an extension of the method treated in Ref. 2 which applies to a three-dimensional central problem. In such a case one has to solve the radial SE

$$\left\{\frac{d^2}{dx^2} + \epsilon - \frac{l(l+1)}{x^2} - V(x)\right\}\psi(x,\epsilon) = 0$$

TABLE II. The BSE for the central potential $V(r) = -400\exp(-r^2)$. l is the orbital quantum number, n is the order of the level for a given l. For simplicity we write, e.g., $52.143\binom{57}{61}$ instead of $^{52.143\,57}_{52.143\,61}$.

$-\epsilon_{nl}$	Present work: the bounds on the BSE	Ref. 11	Ref. 12
$-\epsilon_{50}$	$^{94.457\,68}_{94.457\,76}$	94.457 747 55	94.4577
$-\epsilon_{60}$	$52.143\binom{57}{61}$	52.143 5864	52.1436
$-\epsilon_{70}$	$19.966\binom{28}{30}$	19.966 318	19.9663
$-\epsilon_{80}$	$1.347\,34\binom{2}{4}$	1.347 3	1.3467
$-\epsilon_{71}$	$8.083\,3\binom{27}{32}$	8.083 33	8.0833
$-\epsilon_{72}$	$0.204\,318\binom{8}{9}$	0.204 9	0.1841
$-\epsilon_{63}$	$5.673\,18\binom{2}{7}$	5.673 144	5.6729
$-\epsilon_{54}$	$14.851\,4\binom{8}{9}$	14.851 4875	14.8515
$-\epsilon_{55}$	$1.297\,01\binom{8}{9}$	1.296 99	1.2949

for $x \in (0, \infty)$, $l = 0,1,2,...$, with the boundary conditions

$$\psi(0,\epsilon) = \psi(\infty,\epsilon) = 0.$$

To find the BSE one can employ the phase function $z_R(x,\epsilon)$ satisfying the equations

$$z_R' = (l+1)\cos^2 z_R + (l+1)^{-1}(\epsilon - \tilde{V}(x))\sin^2 z_R,$$
$$z_R(0,\epsilon) = 0,$$
$$z_R'(0,\epsilon) = 1,$$

where $\tilde{V}(x) = l(l+1)/x^2 + V(x)$. The bounds on BSE can be obtained according to the prescription given for the case (B) discussed in the present paper (for details see, e.g., Refs. 2 and 10). To give comparison with some recently reported BSE values[11,12] we have calculated the bounds on the BSE for the three-dimensional central problem with the potential

$$V(x) = -400\exp(-x^2). \tag{A2}$$

In Table II we show our calculated bounds on the BSE together with the results given in Refs. 11 and 12 for several values of l. Except for the case $l = 0$ we show the bounds on the highest BSE given in Ref. 11, some of which were considered unresolved owing to differences between the values presented in Ref. 11 and in Ref. 12. It should be remarked that we did not encounter difficulties with energies lying near the continuum.

APPENDIX B: THEOREMS ABOUT THE ASYMPTOTIC BEHAVIOR OF SOLUTIONS OF EQ. (1.1)

Theorem B1: Let $w(x)$, ϵ in Eq. (1.1) have the properties P. Then there exist positive constants κ, x_0, K, L, and a fundamental system of solutions $\psi_1(x,\epsilon)$, $\psi_2(x,\epsilon)$ of Eq. (1.1) such that for $x > x_0$

$$|\psi_1(x,\epsilon)| \geqslant K\exp(\kappa x), \tag{B1}$$

$$|\psi_2(x,\epsilon)| \leqslant L \exp(-\kappa x). \tag{B2}$$

■

The proof of Theorem B1 given below is sketched in Ref. 13 and carried out in Ref. 5. In the rest of this appendix we assume ϵ to be fixed (having the properties P) and drop writing explicitly the ϵ-dependence of the considered functions. We start with several auxiliary lemmas.

Lemma B1: Let $w(x)$, ϵ in Eq. (1.1) have the properties P. Then there exist $\kappa > 0$, $x_0 > 0$ such that for $x > x_0$

$$w(x) - \epsilon \geqslant \kappa^2. \tag{B3}$$

■

The proof follows directly from the properties P.

Lemma B2: Let $w(x)$, ϵ in Eq. (1.1) have the properties P and $\kappa > 0$, $x_0 > 0$ be the same as in Lemma B1. Consider the solutions u_1, u_2 of Eq. (1.1) such that

$$u_1(x_0) = u_2'(x_0) = 1, \qquad u_1'(x_0) = u_2(x_0) = 0. \tag{B4}$$

Then (1) u_1, u_2 are linearly independent; (2) for $x > x_0$ the following inequalities are valid:

$$u_1(x) \geqslant \cosh \kappa(x - x_0), \qquad u_2(x) \geqslant [\sinh \kappa(x - x_0)]/\kappa. \tag{B5}$$

■

Proof: (1) For the Wronskian of u_1, u_2 it holds $W(u_1,u_2) \equiv 1$, which implies the linear independence of u_1, u_2.

(2) Consider the solutions $g_1(x)$, $g_2(x)$ of the equation

$$g'' - \kappa^2 g = 0 \tag{B6}$$

satisfying (B4) with $u_1 \to g_1$, $u_2 \to g_2$. Then

$$g_1(x) = \cosh \kappa(x - x_0), \qquad g_2(x) = (1/\kappa) \sinh \kappa(x - x_0). \tag{B7}$$

After some simple manipulations with Eqs. (1.1) and (B6) for $x > x_0$ one finds

$$g_i(x)/g_i'(x) \geqslant u_i(x)/u_i'(x) > 0, \tag{B8}$$

for $x > x_0$, $i = 1,2$. Integrating these inequalities and using (B7) one easily obtains (B5).

Let us now consider functions $F(x)$, $G(x)$ defined by the following relations:

$$F(x) = u_1(x)/u_2(x), \tag{B9}$$

$$G(x) = u_1'(x)/u_2'(x), \tag{B10}$$

where $\{u_1,u_2\}$ is the fundamental system of solutions of Eq. (1.1) introduced in Lemma B2.

Lemma B3: Let $F(x)$, $G(x)$ be defined by Eqs. (B9), (B10). Then there exists a constant α, $0 < \alpha < \infty$, such that

$$\lim_{x \to \infty} F(x) = \lim_{x \to \infty} G(x) = \alpha, \tag{B11}$$

$$F(x) > \alpha, \quad F'(x) < 0, \quad \text{if } x > x_0, \tag{B12}$$

$$G(x) < \alpha, \quad G'(x) > 0, \quad \text{if } x > x_0. \tag{B13}$$

■

Proof: The relations (B11)–(B13) can be obtained using the relations (B9) and (B10), by means of which the $F(x)$, $G(x)$ are defined, and the properties of the functions $u_1(x)$, $u_2(x)$ for $x > x_0$.

Now we are ready to prove Theorem B1. A general solution ψ of Eq. (1.1) can be written in the form

$$\psi = Au_1 + Cu_2,$$

where u_1, u_2 are the same as in Lemma B2 and A, C are arbitrary constants. Let us consider solutions $\psi_1(x)$, $\psi_2(x)$ of the form

$$\psi_i(x) = A_i u_1(x) + C_i u_2(x), \quad i = 1,2, \tag{B14}$$

for which

$$C_1/A_1 \neq -\alpha, \qquad C_2/A_2 = -\alpha, \tag{B15}$$

where α is defined by the relation (B11). Then, it follows from Lemmas B2 and B3 that $\psi_1(x)$, $\psi_2(x)$ defined by (B14) and (B15) satisfy (B1) and (B2).

Consider now the function $v(x,\epsilon)$ defined by Eq. (1.4). We shall prove the following theorem.

Theorem B2: Let $w(x)$, ϵ in Eq. (1.1) have the properties P and $v(x)$ be defined by Eq. (1.4) for a solution $\psi(x)$ of Eq. (1.1). Then there exists $\lim_{x \to \infty} v(x) = v(\infty)$ and it holds

$$v^2(\infty) = (w(+\infty) - \epsilon)^{-1}, \quad \text{if } w(+\infty) < +\infty, \qquad v^2(\infty) = 0, \quad \text{if } w(+\infty) = +\infty. \tag{B16}$$

For a solution $\psi(x) \equiv \psi_1(x)$ of Eq. (1.1) satisfying (B1) the function $v(x)$ is positive for sufficiently large x. For a solution $\psi(x) \equiv \psi_2(x)$ satisfying (B2) the function $v(x)$ is negative for sufficiently large x.

■

In the proof of Theorem B2 we shall need the following lemma.

Lemma B4: Let $\psi(x,\epsilon)$ be a solution of Eq. (1.1) with $w(x)$, ϵ having the properties P. Then for sufficiently large x the derivative $\psi'(x)$ satisfies the condition $\psi'(x) \neq 0$.

■

Proof: Let x_0, $u_1(x)$, $u_2(x)$ be the same as in Lemma B2. $\psi'(x)$ can be written in the form

$$\psi'(x) = Au_1'(x) + Cu_2'(x).$$

For $x > x_0$ it holds $u_2'(x) > 0$ and the above relation may be rewritten as

$$\psi'(x) = u_2'(x)\{A\,[u_1'(x)/u_2'(x)] + C\}. \tag{B17}$$

Then, using (B13) and (B17) one can obtain Lemma B4.

Finally, let us prove Theorem B2. The function $v(x)$ satisfies the equation

$$v' = 1 - (w - \epsilon)v^2. \tag{B18}$$

Using (B18), Lemma B4, and the fact that $w(x)$ is continuous for sufficiently large x, one can prove (B16) in full analogy with the proof of Lemma 2.4 in Ref. 2. The last two statements of Theorem B2 can be then obtained by the help of the relations (B14) and (B15), and Lemmas B2 and B3.

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On charges of massless particles

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(Received 15 March 1983; accepted for publication 15 June 1984)

We are concerned with the theorem of Weinberg and Witten stating that a massless particle of helicity $|h| > \frac{1}{2}$ cannot be a carrier of a charge of an internal symmetry induced by a Lorentz covariant current and that for a massless field theory of $|h| > 1$ a Lorentz covariant energy momentum tensor cannot be constructed. We complete the proof of the theorem, as that given by Weinberg and Witten it is inconclusive. We suggest how to evade the difficulties which arise as a consequence of this theorem.

PACS numbers: 03.70. + k, 11.10. − z, 11.40.Dw, 11.30.Cp

I. INTRODUCTION

It has been known for a long time that the case of massless particles of higher helicity causes some serious problems as far as the standard structure of the theory is concerned. The difficulties in constructing the energy-momentum tensor for massless particles of helicity $\frac{3}{2}$ were pointed out, e.g., as early as in 1966 by Bender and McCoy.[1] Recently a paper of Weinberg and Witten[2] devoted to the problem of charges of massless particles elicited considerable interest among physicists and initiated a series of publications on these topics.[3] This paper is also concerned with the "no go" theorem of Weinberg and Witten[2] and consequences following from it. In this theorem it is asserted that a massless particle of helicity $|h| > \frac{1}{2}$ cannot be a carrier of a charge of an internal symmetry induced by a Lorentz covariant current and that for a massless field theory $|h| > 1$ a Lorentz covariant energy momentum tensor cannot be constructed. The proof presented in Ref. 2 is inconclusive as was pointed out by Sudarshan and corroborated by Flato *et al.*[3] in their study; the arguments presented in Ref. 3, however, neither prove nor disprove the statement. Our task, in this paper, will be on one hand to complete the proof of Ref. 2, and on the other hand to show how to evade the difficulties arising as a consequence of this theorem.

The setting for which the theorem is valid is the standard relativistically covariant local quantum field theory in a separable Hilbert space of positive definite metric. In particular, one assumes the spectral condition to be valid and one expects the fields as well as the one-particle states to be operator- or vector-valued distributions, respectively.[4] We want to emphasize that the relativistic covariance, locality, positive definiteness of the metric in the Hilbert space as well as the existence of the one-particle states are crucial for the proof.

The theorem is not true for gauge theories with indefinite metric in the Hilbert space; it is, however, plausible that it is true for the domain of physical states with positive definite metric (see Kugo[3]).

Surprisingly enough the theorem does not exclude the existence of global charges, Lorentz covariant generators of the internal and geometrical symmetries (translations, Lorentz transformations, dilatations, special conformal transformations, supersymmetric charges). They cannot, however, be expressed for higher values of the helicity of the fields concerned as a three-dimensional integral over a time component of a current $j_{N0}(x)$; in other words they are not so-called Noetherian charges for which the following formula holds true[5]:

$$B_N = \int d^3x\, j_{N0}(x)\,; \tag{1.1}$$

here B_N denotes a charge, N stands for any set of Lorentz (spinor or tensor) indices, and the current $j_{N\mu}(x)$ ($\mu = 0,1,2,3$) is a Poincaré covariant local field which is a locally conserved quantity, viz.

$$\partial^\mu j_{N\mu}(x) = 0\,. \tag{1.2}$$

Of course, they may but do not need to exist. It is known, e.g., from the investigation of Refs. 6 that in electrodynamics of photons and electrons the existence of an electric charge operator entails spontaneous breakdown of the Poincaré symmetry of the theory as a consequence of the Gaussian law. This does not, however, apply to free fields for which all the before-mentioned global charges can be explicitly constructed as well-defined operators. Nevertheless, even in the free field case the theorem prevents the existence of currents satisfying (1.1) and (1.2).

To resolve this problem the following observations are in order.

First of all, the procedure proposed in Ref. 2 does not exclude for higher values of helicity of the fields concerned with the existence of Lorentz covariant currents which—being the carriers of a charge—compulsory change the sign of the helicity while acting upon a one-particle state. This fact was observed by Sudarshan in his paper.[3] This effect seems at first glance to be in contradiction with the Coleman Mandula "no go" theorem[7] in the case of an interacting field theory. This does not need to be so, however, as (1) the change of a sign of helicity is related to a discrete symmetry (space reflection) to which the Coleman Mandula theorem does not apply; (2) the Coleman Mandula theorem was proven only in case of massive particles; and (3) to preserve the locality of the fields we have to always combine two terms of opposite helicity.

What is even more important is that the procedure of Ref. 2 does not exclude the existence of currents which are nonlocal or nonlocal and noncovariant with respect to the

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 0022-2488/84/123503-07$02.50

Lorentz transformations. There can exist[8] operator densities, sesquilinear in the creation and annihilation operators of massless particles with almost parallel momenta which yield finite, nonvanishing contribution when integrated over three-dimensional x-space. These densities, however, do not transform under the Lorentz transformation as the time component of a four-vector and are not local. Another, rather natural, way out closer to the intuitions inherited from classical physics are currents constructed out of potentials of the fields rather than out of the fields themselves. It can be shown that such currents give rise, according to (1.1), to Lorentz covariant charges. These currents are also nonlocal although they are locally conserved.

II. THE METHOD OF WEINBERG AND WITTEN

Following the method proposed by Weinberg and Witten[2] we are going to investigate the properties of the matrix elements

$$(\psi(p;h),\Phi_N(x)\psi'(p';h')) \tag{2.1}$$

for[9] $(p-p')^2<0$, where $\psi(p;h)$ and $\psi'(p',h')$ denote any massless one-particle states characterized by momentum p or p' ($p^2=p'^2=0$, $p_0\geqslant 0$, $p_0'\geqslant 0$) and helicity h or $h'=0, \pm\frac{1}{2}, \pm 1,\ldots$, respectively, and $\Phi_N(x)$ is any translationally covariant quantum field whose Lorentz transformation properties are characterized by the tensor, spinor, or tensor–spinor index N[4], viz.

$$U(A,a)\Phi_N(x)U(A,a)^+=\sum_M (S^{-1})_N{}^M\Phi_M(\Lambda x+a)\,. \tag{2.2}$$

Here $U(A,a)$ is a unitary operator representing in the Hilbert space the element of the Poincaré group characterized by $A\in SL(2,C)$, i.e., $A=\left(\begin{smallmatrix}\alpha&\beta\\ \gamma&\delta\end{smallmatrix}\right)$; $\alpha\delta-\beta\gamma=1$, $\alpha,\beta,\gamma,\delta$-complex numbers and $a\equiv(a_0,a_1,a_2,a_3)$, $a_\mu=\bar a_\mu$, $S_N{}^M=S(A)_N{}^M$ represents the same group element A in a space of dimension determined by the tensor character of the field (indicated by the index N), finally $\Lambda^\nu_\mu=\Lambda(A)^\nu_\mu$ is the four-dimensional Lorentz transformation corresponding to A. The reason for a careful examination of (2.1) is that, as far as the symmetries are concerned, the physically most interesting quantities like charges or currents which give rise to these charges have to exert a nontrivial action upon the one-particle Hilbert space. Should, e.g., a symmetry leave intact the one-particle states corresponding to a certain field, this would imply that the field itself is also invariant under these transformations.[10]

To start our considerations let us summarize the transformation properties of the massless one-particle state $\psi(p;h)$.[11] Due to positive definite metric of the Hilbert space, we have

$$U(A,0)\psi(p;h)=\psi(\Lambda p;h)\exp\{ih\nu\}\,, \tag{2.3}$$

where $\nu=\nu(A,p)=\bar\nu$ is the so-called Wigner phase. The term $\exp\{ih\nu\}$ is a one-dimensional representation of an element $e(A,p)$ of the little group E_2 (two-dimensional Euclidean motion) of the massless Poincaré group representation. To define $e(A,p)$ we have to first define the Wigner boost transformation $[p]\in SL(2,C)$. To this aim let us write

$$\sigma^\mu_{A\dot B}\,p_\mu\equiv p_{A\dot B}\equiv s_A\,\overline{s_B}\,,\quad A,B=1,2\,, \tag{2.4}$$

where s_A, $A=1,2$, transform as spinor components. This is possible due to $p_{1\dot 1}\geqslant 0, p_{2\dot 2}\geqslant 0, p_{1\dot 2}=\overline{p_{2\dot 1}}$, and $p^2=0$. In (2.4)

$$\sigma^0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma^1=\begin{pmatrix}0&1\\1&0\end{pmatrix},$$
$$\sigma^2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma^3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

From the multitude of boost transformations which transform the pseudovector

$$\hat p=r(1,0,0,1)\,,\quad r>0$$

or

$$\hat p_{A\dot B}=\rho^2\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad \rho^2\equiv 2r$$

into a massless p_μ, $\mu=0,1,2,3$, or $p_{A\dot B}=s_A\,\overline{s_B}$, we choose one which best suits our goal (valid for $p_0+p_3\neq 0$) viz.

$$[p]_B{}^C=\begin{pmatrix}\dfrac{|s_1|}{\rho}, & 0\\ \dfrac{s_2}{\rho}\dfrac{\bar s_1}{|s_1|}, & \dfrac{\rho}{|s_1|}\end{pmatrix}. \tag{2.5}$$

The inverse transformation reads

$$[p]^{-1}{}_B{}^C=\begin{pmatrix}\dfrac{\rho}{|s_1|}, & 0\\ -\dfrac{s_2}{\rho}\dfrac{\bar s_1}{|s_1|}, & \dfrac{|s_1|}{\rho}\end{pmatrix}. \tag{2.6}$$

With the help of (2.5) and (2.6) we may define

$$e(A,p)\equiv[\Lambda p]^{-1}A\,[p]\in E_2 \tag{2.7}$$

which, for our special choice of boosting, reads

$$e(A,p)=\frac{1}{|\tilde s_1|\,|s_1|}\begin{pmatrix}\bar s_1\tilde s_1 & \rho^2\beta\\ 0 & s_1\bar{\tilde s}_1\end{pmatrix},$$

where

$$\tilde s_1\equiv\alpha s_1+\beta s_2\,,\quad \tilde s_2\equiv\gamma s_1+\delta s_2\,.$$

It can be shown that its one-dimensional representation

$$e\{ih\nu\}$$

is linked to the (λ,λ)-term ($\lambda=h+|h|+1$) of the $(2h+1)$-dimensional triangle matrix representation $\mathscr{D}^{(|h|,0)}(e^{-1})$ of the inverse of the element e given by (2.7) by

$$\mathscr{D}^{(|h|,0)}(e^{-1})_{\lambda,\lambda}=e^{ih\nu}=\left(\frac{\alpha+\beta(s_2/s_1)}{|\alpha+\beta(s_2/s_1)|}\right)^{2h}. \tag{2.8}$$

Let us examine the transformation properties of the expression (2.1). We find that in virtue of (2.2) and (2.3)

$$\begin{aligned}&(\psi(p;h),\Phi_N(x)\psi'(p';h'))\\ &\quad=(U(A,0)\psi(p;h),U(A,0)\Phi_N(x)\psi'(p';h'))\\ &\quad=\exp\{-i(h\nu(A,p)-h'\nu(A,p'))\}\\ &\qquad\times\sum_M(S^{-1})_N{}^M(\psi(\Lambda p;h),\Phi_M(\Lambda x)\psi(\Lambda p';h'))\,.\end{aligned} \tag{2.9}$$

Let us now, following Weinberg and Witten, take as A the three-dimensional rotation through the angle Θ around the axis pointing in the direction $\mathbf{q}$, viz.

$$\mathring A=\sigma^0\cos\frac{\Theta}{2}+i\sin\frac{\Theta}{2}\sum_{j=1}^3\sigma^j\cos\phi_j\,, \tag{2.10a}$$

$$\cos\phi_j = \pm\frac{q_j}{q_0},\quad j=1,2,3,\quad q_0 = +\left(\sum_{j=1}^{3} q_j^2\right)^{1/2}. \tag{2.10b}$$

For such a transformation

$$q = \mathring{A}q \tag{2.11}$$

and, in virtue of (2.5)–(2.7) and (2.10)–(2.11) we get

$$\mathscr{D}^{(|h|,0)}(\mathring{e}^{-1})_{\lambda,\lambda} = \exp\{\pm i\Theta/2\},$$
$$\lambda = h + |h| + 1,\quad h = -\tfrac{1}{2},\tfrac{1}{2}. \tag{2.12}$$

This formula can be extended to an arbitrary half-integer h by using (2.8).

Thus we infer from (2.12) that for $A = \mathring{A}\,\nu$ appearing in (2.3) or (2.8) coincides up to the sign with the angle of rotation Θ, $\Theta = \pm\nu(\mathring{A},q)$. Again following Weinberg and Witten we may choose a special Lorentz frame of reference in which the momenta appearing in (2.9) satisfy the relation

$$\mathbf{p} + \mathbf{p}' = 0,\quad p_0 + p_0' = 2|\mathbf{p}|. \tag{2.13}$$

We may also choose as a Lorentz transformation in (2.9) the transformation $\mathring{A}$ given by (2.10) taken for $\mathbf{q} = \mathbf{p}$; then

$$\Theta = \nu(\mathring{A}, p) = -\nu(\mathring{A}, p'). \tag{2.14}$$

Moreover, due to (2.11)

$$\mathring{A}\,p = p,\quad \mathring{A}\,p' = p'. \tag{2.15}$$

Taking into account (2.13)–(2.15) we get from the relation (2.9) that

$$\phi_N(p,p';h,h') = \exp\{-i(h+h')\Theta\}\sum_M (\mathring{S}^{-1})_N{}^M \Phi_M(p,p';h,h'), \tag{2.16}$$

where we used the shorthand notation

$$(\psi(p;h),\Phi_N(x)\psi'(p';h')) \equiv \Phi_N(p,p';h,h')e^{i(p-p')x}. \tag{2.17}$$

Formula (2.16) is the main object of our investigation. In the next section we shall examine (2.16) for different kinds of fields and discuss conclusions drawn from it. In particular, we shall give the proof of the theorem of Weinberg and Witten[2] somewhat extended by us. The crucial point will be that the right-hand side of (2.16) depends on Θ while the left-hand side does not.

III. PROOF OF THE THEOREM OF WEINBERG AND WITTEN

Let us examine Eq. (2.16) and the conclusions resulting from it.

The simplest case is when field $\Phi_N(x)$ is a scalar field, i.e.,

$$\Phi_N(x) \equiv \phi(x).$$

For this case Eq. (2.16) reduces to

$$\Phi(p,p';h,h') = \exp\{-i(h+h')\Theta\}\Phi(p,p';h,h'),$$

which implies for any Lorentz frame of reference

$$\Phi(p,p';h,h') = 0 \quad \text{for } |h+h'|>0 \text{ and } (p-p')^2<0, \tag{3.1}$$

in particular,

$$\Phi(p,p';h,h) = 0 \quad \text{for } |h|>0 \text{ and } (p-p')^2<0. \tag{3.2}$$

For $h + h' = 0$ and $h \neq 0$, the expression $\Phi(p;p',h,-h)$ does not need to vanish. This means that there are scalar fields which may change the sign of helicity when applied to a one-particle state; notice that this set of fields is not empty.

In a similar way as in the case of scalar fields, it follows from (2.16) that $\Phi_N(p,p',h,h')$ defined by (2.17) vanishes for $(p-p')^2<0$, where

$$\begin{aligned}&\Phi_N(x) \text{ is a spinor field and } |h+h'|\neq\tfrac{1}{2},\\ &\quad\text{a vector field and } |h+h'|\neq 0 \text{ or } 1,\\ &\quad\text{a Rarita–Schwinger field and } |h+h'|\neq\tfrac{1}{2} \text{ or } \tfrac{3}{2},\\ &\quad\text{a second rank tensor field and } |h+h'|\neq 0 \text{ or } 1 \text{ or } 2.\end{aligned} \tag{3.3}$$

We list here the main results shifting most of the computations to the Appendix.

Weinberg and Witten claim that (3.1) or (3.3) imply the vanishing of these matrix elements also for $(p-p')^2 = 0$ by continuity. Unfortunately, their statement is incorrect as the continuity with respect to the particle momenta cannot be proven, which was pointed out by Sudarshan and Flato *et al.*[3] What follows from (3.1) and (3.3) for sure is that

$$\Phi(p,p';h,h') = g(\mathbf{p},\mathbf{p}';h,h')D\delta(\mathbf{n},\mathbf{n}'), \tag{3.4}$$

where $\mathbf{n}$ and $\mathbf{n}'$ are unit vectors pointing in the direction $\mathbf{p}$ and $\mathbf{p}'$, respectively. $\delta(\mathbf{n},\mathbf{n}')$ denotes the delta-function on the unit sphere and D is a polynomial in the angle derivatives of $\mathbf{n}$ on the sphere. This expression when multiplied by $\exp\{i(p-p')\}$ and integrated[5] over $\mathbf{x}$ may yield a physically reasonable result. A neat example[8] is

$$\frac{(p_0-p_0')^2}{(p_0p_0')^{1/2}}\delta(\mathbf{n},\mathbf{n}')e^{ix(p'-p)};\quad p_0 \equiv |\mathbf{p}|. \tag{3.5}$$

In view of the relation

$$\lim_{R\to\infty}\int d^3x f\left(\frac{|\mathbf{x}|}{R}\right)e^{-ix(\mathbf{p}-\mathbf{p}')}\frac{(p_0-p_0')}{2p_0p_0'}\delta(\mathbf{n},\mathbf{n}') = 2\pi^2 f(0)\delta(\mathbf{p}-\mathbf{p}'), \tag{3.6}$$

this expression leads to a "charge" whose kernel on the one-particle space is given by

$$2p_0\delta(\mathbf{p}-\mathbf{p}').$$

This is what one would expect from a genuine generator of an internal symmetry.

Notice, however, that (3.5) does not transform under Lorentz transformations like the time component of a four-vector (as required by the assertion of Weinberg and Witten) but as the $\mu=\nu=\rho=0$ component of a rank 3 tensor $\Phi_{\mu\nu\rho}$. This "wrong" connection between the transformation properties of charges and currents leading to form factors of the type (3.4) is a quite general feature. To make this plain let us

discuss the case where $h = h'$ and $D = 1$ in (3.4). It follows from the scale invariance of the Wigner phases [cf. relation (2.8)] and the fact that

$$\frac{1}{p_0 p_0'}\,\delta(\mathbf{n},\mathbf{n}')$$

is a Lorentz-invariant kernel that these form factors can be represented by

$$(\psi(p,h),\Phi_{N\mu}\psi(p',h)) = T_{N\mu}(p,\lambda)\cdot(1-\lambda)(1-\lambda^{-1}) \times(\delta(\mathbf{n},\mathbf{n}')/p_0 p_0')\cdot e^{ix(p-p')}. \quad (3.7)$$

Here $\lambda = p_0'/p_0$ and $T_{N\mu}(p,\xi)$ is (for fixed ξ) a covariant tensor satisfying the continuity equation $p^\mu T_{N\mu}(p,\xi) = 0$. Using relation (3.6) we thus obtain for the matrix elements of the corresponding charge the expression

$$(\psi(p,h), B_N\psi(p',h)) = (2\pi/p_0)^3\cdot T_{\mathrm{No}}(p,1)\cdot 2p_0\delta(\mathbf{p}-\mathbf{p}'). \quad (3.8)$$

But $(1/p_0^3)T_{\mathrm{No}}(p,1)$ is clearly not a Lorentz-covariant tensor of type N. The generalization of this argument to the case $D \neq 1$ is technically tedious but ideologically straightforward. So we arrive at the following, somewhat extended version of the theorem of Weinberg and Witten.

Theorem: A massless particle of helicity h, $|h| > \frac{1}{2}(j+k)$, cannot be a carrier of a Poincaré covariant charge induced by a covariant current $\Phi^{(j,k)}(x)$ in a way indicated in (1.1), where j and $k = 0,\frac{1}{2},1,\ldots$, indicate the transformation character of the field with respect to the Lorentz group.

Let us remark[12] that currents leading to form factors of the singular type (3.4) cannot be local. In local field theory it can be shown that any charge B_N which is obtained[5] from a local, covariant current $\Phi_{N,\mu}$ is covariant. Assuming that a dense set of single particle states is in the domain[13] of B_N, this fact is, as we have seen, not compatible with a behavior of the currents as in (3.4). A more direct way of seeing that these currents are dislocalized is the following one: If one replaces f in relation (3.6) by a test function which is not spherically symmetric, then relation (3.6) no longer holds. Therefore, the matrix elements

$$(\psi_{\mathrm{loc}}, \Phi_{\mathrm{No}}(\mathbf{x},f_T)\psi_{\mathrm{loc}}')$$

cannot be rapidly decreasing if $|\mathbf{x}|$ tends to infinity, unless they are identically zero. This leads to the following result under the above mild domain assumptions.

Corollary: In a local field theory one gets under the assumptions of the previous theorem

$$(\psi(p,h),\Phi^{(j,k)}(x)\psi(p;h)) = 0.$$

Thus the "continuity assumption" of Weinberg and Witten is a consequence of locality.

These results seem to be at first glance extremely restrictive and strange, as they hold true for each field irrespectively of whether it interacts or not. On second thought, however, we conclude that the situation is not so dramatic; we are going to make things clearer in Sec. V.

IV. OTHER CONCLUSIONS

The theorem does not exclude the existence of nonlocal fields whose matrix elements (3.4) are concentrated on the light cone $(p-p')^2 = 0$. In particular, all fields which satisfy

$$[\cdots[[\Phi_N(x),P_{\lambda_1}]P_{\lambda_2}]\cdots P_{\lambda_s}] = 0,$$
$$\lambda_j = 0,1,2,3,\ s-\text{finite},\ \text{integer} > 0 \quad (4.1)$$

may have nonvanishing matrix elements in the close neighborhood of $(p-p')^2 = 0$. The link between (3.4) and (4.1) is provided by the formula

$$(1/n!)x^n\,\partial^n\delta(x) = (-1)^n\delta(x).$$

Every generator of an internal symmetry (i.e., a Poincaré invariant operator), generators of translations P_μ, Lorentz generators

$$M_{\mu\nu}(x) = e^{iPx}M_{\mu\nu}e^{-iPx} = M_{\mu\nu} - x_\mu P_\nu + x_\nu P_\mu,$$

generator of dilations

$$D(x) = D - x^\lambda P_\lambda,$$

and special conformal transformations

$$K_\mu(x) = K_\mu - 2(x_\mu D + x^\lambda M_{\mu\lambda}) + (2x_\mu x^\nu P_\nu - x^2 P_\mu)$$

as well as the generators of the supersymmetry of the first and second kind, Q_B, Q_B^+ and S_B, S_B^+, respectively, fall into this class. According to O'Reifeartaigh's theorem,[14] every generator of a group of finite order satisfies (4.1) provided we have one-particle states in the theory.

For $|h+h'| = \frac{1}{2}$, nontrivial spinor and Rarita–Schwinger fields $\Phi_N(x)$ may exist; we call a field nontrivial when it does not satisfy relations like (3.4). Even then the spinor field $\Phi_N(x) = \Phi_A^{(1/2,0)}(x)$ has to satisfy the subsidiary conditions

$$p^{A\dot{B}}\Phi_A(p,p';h,h') = 0 \quad \text{for } h+h' = -\tfrac{1}{2} \quad (4.2a)$$

and

$$p'^{A\dot{B}}\Phi_A(p,p';h,h') = 0 \quad \text{for } h+h' = \tfrac{1}{2}, \quad (4.2b)$$

Notice that these are not Weyl equations. Incidentally, relations (4.2) prevent the locally conserved current

$$j_{C\dot{A}B}(x) \equiv \epsilon_{A\dot{B}}\Phi_C(x), \quad \epsilon \equiv i\sigma^2, \quad (4.3)$$

to give rise to a supersymmetric charge. The argument is based upon the fact that local conservation of (4.3) implies that $\Phi_C(x)$ satisfies the Weyl equation

$$(p^{A\dot{B}} - p'^{A\dot{B}})\Phi_A = 0. \quad (4.4)$$

More details can be found in the Appendix. Also the current

$$j_{C\dot{A}B}(x) = \partial_{A\dot{B}}\Phi_C(x)$$

cannot be used as a supersymmetric current. Of course, the case where Φ_A is a free field[15] is trivially excluded.

The Rarita–Schwinger field $\phi^{(1,1/2)}(x)$ [or $\phi^{(1/2,1)}(x)$] is subject to similar restrictive conditions as (4.2). In the latter case, the supersymmetric charge induced by a current can be carried only by particles of $h = 0, \pm\frac{1}{2}$ or ± 1; this follows from the observations that the supersymmetric charge acting on a one-particle state changes its helicity by $\pm\frac{1}{2}$. For $h > 1$, only global supersymmetric generators, which cannot be presented in the form (1.1), may exist.

For $|h+h'| = 1$, the vector field $\phi_{A\dot{B}}^{(1/2,1/2)} = \sigma_{A\dot{B}}^\mu V_\mu$ has to be necessarily locally conserved when applied in the one-particle Hilbert space.

Let us finally look at the second rank tensor field $\phi_{ABCD}^{(1,1)} = \sigma_{AC}^\mu\sigma_{BD}^\nu T_{\mu\nu}$ and concentrate upon the most interesting case $h = h' = \pm 1$. Then, $\Phi_{\mu\nu}(p,p',\pm 1,\pm 1) = \Phi_{\mu\nu}$ is necessarily locally conserved and traceless, viz.

$$(p-p')^{\mu}\Phi_{\mu\nu}=(p-p')^{\nu}\Phi_{\mu\nu}=0\,,$$
$$\Phi^{\mu}{}_{\mu}=0\,. \tag{4.5}$$

If $\Phi_{\mu\nu}$ is skew symmetric then $\Phi_{\mu\nu}$ and its dual $\tilde{\Phi}_{\mu\nu}=(i/2)\epsilon_{\mu\nu\kappa\lambda}\Phi^{\kappa\lambda}$ satisfy all Maxwell equations and, consequently, the d'Alembert equation.

If $\Phi_{\mu\nu}$ is skew symmetric and, in addition, self- or antiself-dual, viz.

$$\tilde{\Phi}_{\mu\nu}=\pm\Phi_{\mu\nu}\,,$$

then $\Phi_{\mu\nu}=0$. This was to be expected from the considerations of the vector case; there we showed that $\Phi_{\dot{A}\dot{B}}^{(1/2,1/2)}=0$ for $|h|>\frac{1}{2}$; this should imply $\Phi_{AB}^{(1,0)}=\Phi_{\dot{A}\dot{B}}^{(0,1)}=0$ for $|h|>\frac{1}{2}$ too.

The most interesting case of a symmetric tensor $T_{\mu\nu}$ is the case of the energy-momentum tensor $S_{\mu\nu}$. This tensor has to be locally conserved and can be made symmetric. However, not always can one remodel it so that its trace vanishes. If the examined field theory is dilatationally covariant then either the fields have canonical dimensions and in consequence of that are free massless fields or the dimension is anomalous and we have to do with interacting fields which, however, do not admit particle interpretation.[16] In our presentation, the existence of massless one-particle states is explicitly assumed. This implies either a free, dilatationally covariant, massless field theory or a theory of dilatationally noncovariant interacting fields which admit massless particle interpretation. In the first case, the energy-momentum tensor can be made traceless. In the latter case, the dilatation current

$$D_{\mu}(x)\equiv x^{\lambda}S_{\lambda\mu}(x) \tag{4.6}$$

is no longer locally conserved and

$$S^{\mu}{}_{\mu}(x)=\partial^{\mu}D_{\mu}(x)\neq 0\,.$$

In our investigation we are interested in matrix elements

$$(\psi(p;h),S_{\mu\nu}(0)\psi'(p';h))\,,$$

where $\psi(p;h)$ are massless one-particle states; in this case we may always find such $S_{\mu\nu}$ that (4.5) holds.

Taking into account the considerations presented above, the following problem arises. Since for the massless particles with $|h|>1$ an energy-momentum tensor cannot be constructed this implies that standard dilational, conformal as well as Lorentz transformation currents also do not exist. The standard dilational current is given by (4.6), the conformal one reads

$$K_{\mu\nu}(x)=x^2S_{\mu\nu}(x)-2x_{\nu}x^{\lambda}S_{\lambda\mu}(x)\,,$$

where $S_{\mu\nu}$ is the locally conserved, symmetric and traceless energy-momentum tensor.

We are going to show in the next section how to solve this dilemma.

V. HOW TO EVADE THE DIFFICULTIES CREATED BY THE THEOREM OF WEINBERG AND WITTEN

(i) The following example shows that there can exist local, Lorentz covariant, Hermitian currents which preserve the absolute value of the helicity but not the helicity itself. This fact was noticed earlier by Sudarshan.[3]

Let us examine the current.

$$j_{\lambda}(x)=i:\{F^{\mu\nu}(\partial_{\lambda}F^{+}_{\mu\nu})-(\partial_{\lambda}F^{\mu\nu})F^{+}_{\mu\nu}\}:(x)\,,$$

where $F_{\mu\nu}=-F_{\mu\nu}$ is a free local massless tensor field; in addition we require that $F_{\mu\nu}$ is neither self- or antiself-dual and $F_{\mu\nu}\neq(F_{\mu\nu})^{+}$. In the spinor notation of van der Waerden we have

$$F_{AB\dot{C}\dot{D}}\equiv\sigma^{\mu}_{A\dot{C}}\sigma^{\nu}_{B\dot{D}}F_{\mu\nu}=S_{AB}\epsilon_{\dot{C}\dot{D}}+A_{\dot{C}\dot{D}}\epsilon_{AB}\,,$$

with

$$S_{AB}\neq 0\,,\quad A_{\dot{C}\dot{D}}\neq 0\,,\quad (S_{AB})^{+}\neq A_{\dot{A}\dot{B}}\,.$$

As $F_{\mu\nu}$ is assumed to be a free local massless field, S_{AB} as well as $A_{\dot{A}\dot{B}}$ can be separated into two Lorentz covariant parts, viz.

$$S_{AB}=S^{(1)}_{AB}(-h)+(S^{(2)}_{AB}(h))^{+}\,,\quad h=1\,,$$
$$A_{\dot{A}\dot{B}}=(A^{(1)}_{AB}(-h))^{+}+A^{(2)}_{\dot{A}\dot{B}}(h)\,,$$

where $S^{(1)}_{AB}(-h)$, $S^{(2)}_{AB}(h)$, $A^{(1)}_{AB}(-h)$, and $A^{(2)}_{\dot{A}\dot{B}}(h)$ are linear in the creation operators. It is easy to see that the nonvanishing contribution obtained from

$$(\psi(p,h),:F_{AB\dot{C}\dot{D}}(F^{+})^{AB\dot{C}\dot{D}}:\psi'(p';h'))$$

arises from terms

$$S^{(1)}(-h)(A^{(2)}(h))^{+}\,,\quad A^{(1)}(-h)(S^{(2)}(h))^{+}\,,$$
$$A^{(2)}(h)S^{(1)}(-h)^{+}\,,$$

and $S^{(2)}(h)(A^{(1)}(-h))^{+}$, i.e., terms with $h=-h'$.

(ii) Another solution to the dilemma is to make use of currents which are noncovariant with respect to the Lorentz transformations. Besides the expressions of type (3.4) discussed before, there exists currents constructed out of potentials of the fields rather than out of the fields themselves as customary in the traditional formalism of classical physics. These currents are locally conserved and give rise to Lorentz covariant charges which do not change momentum and helicity of a one-particle state; these currents are, however, nonlocal.

In a theory of a free local massless skew symmetric and self-dual field $F_{\mu\nu}$ the nonlocal and Lorentz noncovariant current

$$J_{\lambda}(x)=i:\{A^{1}(\partial_{\lambda}A^{+}_{1})-(\partial_{\lambda}A^{1})A^{+}_{1}\}:(x)$$

yields a *bona fide* scalar charge. Here[17]

$$F_{0j}=\partial_0A_j\,,\quad i,j=1,2,3\,,$$
$$F_{ij}=\partial_iA_j-\partial_jA_i\,,$$
$$\partial^{i}A_i=0\,,\quad A_0=0\,,\quad \Box A_i=0\,.$$

A similar procedure can be applied in the theory of a free local massless self-dual field $R_{\kappa\lambda\mu\nu}$ of helicity 2 in constructing the energy-momentum tensor. The field $R_{\kappa\lambda\mu\nu}$ is linked to the Riemannian curvature tensor and to the linearized Einstein gravitation.[18] The nonlocal and Lorentz noncovariant energy-momentum tensor reads

$$S_{\mu\nu}=:\{\partial_{\mu}h^{\kappa\lambda}\partial_{\nu}(h_{\kappa\lambda})^{+}+\partial_{\mu}(h^{\kappa\lambda})^{+}\partial_{\nu}h_{\kappa\lambda}$$
$$-\eta_{\mu\nu}\partial^{\sigma}h^{\kappa\lambda}\partial_{\sigma}h_{\kappa\lambda}\}:(x)\,,$$

where $\eta_{\mu\nu}=\mathrm{diag}(1,-1,-1,-1)$. This energy-momentum tensor yields proper Lorentz covariant generators of the translations and other symmetries linked to the energy-momentum tensor. Here

$$R_{\kappa\lambda\mu\nu} = -\partial_\kappa(\partial_\mu h_{\lambda\nu} - \partial_\nu h_{\lambda\mu}) + \partial_\lambda(\partial_\mu h_{\kappa\nu} - \partial_\nu h_{\kappa\mu}).$$

The potentials $h_{\mu\nu}$ are restricted by the following constraints:

$$h_{\mu\nu} = h_{\nu\mu},$$

$$i\epsilon_{\mu\nu\kappa\lambda}\,\partial^\kappa(\partial^\rho h^{\lambda\sigma} - \partial^\sigma h^{\lambda\rho}) = \partial_\mu(\partial^\rho h^\sigma_\nu - \partial^\sigma h_\nu{}^\rho) - \partial_\nu(\partial^\rho h_\mu{}^\sigma - \partial^\sigma h_\mu{}^\rho),$$

$$\partial^\mu h_{\mu\nu} = \tfrac{1}{2}\partial_\nu h^\kappa{}_\kappa \quad \text{(de Donder gauge)},$$

$$\Box h_{\mu\nu} = 0,$$

$$h_{00} = h_{0j} = 0.$$

The observations made above show that in field theory of massless particles we are forced to introduce into the theory Lorentz noncovariant, gauge-dependent quantities like potentials in electromagnetism or metric tensor in linearized Einstein gravitation to preserve the notion of currents giving rise to conserved Lorentz covariant quantities. This observation is of a general nature as for each massless field of higher-tensor character we may, in virtue of the Bianchi identities and the inverse of the Poincaré lemma, introduce potentials. These potentials transform under the Lorentz transformation noncovariantly, in particular the polarization factor acquires a phase $\exp\{ihv(A,p)\}$. The current is constructed in such a way that it is a sesquilinear form in the potential. When we integrate this current over $\mathbf{x}$ the phases of the two potential operators cancel each other and we get a Lorentz covariant global change.

ACKNOWLEDGMENTS

Discussions with Dr. D. Buchholz, Dr. W. Garczynski, Dr. J. Lukierski, Dr. J. Perk, Dr. K. Pilch, and Dr. S. Rabsztyn are gratefully acknowledged. I am in particular very grateful to the unknown referee of this paper whose contributions essentially improved the substance of it. I would like to express my sincere thanks for the warm hospitality extended to me by Professor C. N. Yang during my stay at the Institute for Theoretical Physics, State University of New York, SUNY at Stony Brook, NY, and by Professor H. Reeh, during my stay at the Institute of Theoretical Physics, University of Göttingen.

Research was partly supported by National Science Foundation Grant No. PHY81-90110 and by the Polish Department Program MR.1.7 for 1983.

APPENDIX

We give here some more information about the cases of spinor, vector and tensor fields.

(*i*) *Case of spinor field*: $\Phi_N(\mathrm{x}) = \Phi_{\mathrm{B}}^{(1/2,0)}$ or $\Phi_{\dot B}^{(0,1/2)}$ $(B = 1,2)$.

According to (2.16) in the special Lorentz frame of reference and for $(p-p')^2 < 0$ we have [Φ_B stands here for $\Phi_B^{(1/2,0)}(p,p';h,h')$ etc.]

$$\Phi_B = \exp\{-i(h+h')\Theta\}\{\mathring{A}^{-1}\}_B{}^C\Phi_C,$$

$$\Phi_{\dot B} = \exp\{-i(h+h')\Omega\}\{\mathring{A}^{-1}\}_{\dot B}{}^{\dot C}\Phi_{\dot C},$$

which after taking into account (2.10) and arbitrariness of the angle θ reduce to (4.2) and complex conjugate of it or yield $\Phi_A = \Phi_{\dot B} = 0$ otherwise.

The relations (4.2) are Lorentz covariant and should hold in any frame of reference.

(*ii*) *Current* $\epsilon_{A\dot B}\Phi_C(x)$: We prove for $h + h' = \frac{1}{2}$ that the current (4.3) does not give rise to a supersymmetric charge. In this case Φ_A satisfies simultaneously (4.2b) and (4.4). The solution to (4.2b) is

$$\Phi_A = \lambda(p,p')p'_{A\mathrm{i}}$$

and (4.4) implies

$$p^{A\dot B}\Phi_A = \lambda(p,p')p^{A\dot B}p'_{A\mathrm{i}} = 0 \tag{A1}$$

for any choice of p and p' when $(p-p')^2 < 0$. In the special frame of reference, $p_0 = p'_0$ $\mathbf{p} = -\mathbf{p}'$ (A1) reads

$$\lambda(p,p')p_{22}(p_{22}+p_{11}) = 0,$$

$$\lambda(p,p')p_{21}(p_{22}+p_{11}) = 0,$$

which should be valid for any choice of p. Therefore, $\lambda(p,p') = 0$ consequently in any frame of reference

$$\Phi_A = 0 \quad \text{for } (p-p')^2 < 0$$

as has to be shown.

(*iii*) *Case of vector field*: $\Phi_N(x) = V_\mu(x) = \frac{1}{2}(\sigma_\mu)^{A\dot B}\phi_{A\dot B}^{(1/2,1/2)}$. This is the case considered in Ref. 2, except that we are not going to assume at the start that it is a current. According to (2.16) we have [Φ_μ stands for $\Phi_\mu(p,p';h,h')$]

$$\Phi_0 = e^{-i(h+h')\Theta}\Phi_0,$$

$$\Phi_k = e^{-i(h+h')\Theta}\sum_{l=1}^{3} R^{-1}_{kl}\Phi_l, \quad k = 1,2,3, \tag{A2}$$

where R is the three-dimensional rotation matrix corresponding to (2.10) or

$$\Phi_k = e^{-i(h+h')\Theta}\left\{\cos\Theta\Phi_k + (1-\cos\Theta)\frac{p_k}{p_0}\frac{p_l}{p_0}\Phi_l + \sin\Theta\epsilon_{klm}\frac{p_l}{p_0}\Phi_m\right\}$$

$$= e^{-i(h+h')\Theta}\frac{p_k}{p_0}\frac{p_l}{p_0}\Phi_l + \tfrac{1}{2}e^{-i(h+h'-1)\Theta}\left\{\Phi_k - \frac{p_k}{p_0}\frac{p_l}{p_0}\Phi_l - i\epsilon_{klm}\frac{p_l}{p_0}\Phi_m\right\} + \tfrac{1}{2}e^{-i(h+h'+1)\Theta}\left\{\Phi_k - \frac{p_k}{p_0}\frac{p_l}{p_0}\Phi_l + i\epsilon_{klm}\frac{p_l}{p_0}\Phi_m\right\}.$$

The only admissible cases are $h + h' = 0$, $+1$ and -1. For $h + h' = 0$ it follows from (A2) that Φ_0 is arbitrary and

$$\Phi_k = \alpha p_k.$$

If we require in addition that Φ_μ is a current we have in this special Lorentz frame of reference

$$p_k\Phi_k = \alpha p_k p_k = 0,$$

which implies for an arbitrary frame of reference that Φ_μ is symmetric with respect to the interchange of p and p', viz.

$$\overline{\Phi}_\mu \sim p_\mu + p'_\mu$$

and therefore, is not a gradient of a scalar.

For $h + h' = \pm 1$ from (A2) follows $\Phi_0 = 0$ (A3a)

$$\Phi_k = \mp i\epsilon_{klm}(p_l/p_0)\Phi_m. \tag{A3b}$$

From (A3) follows immediately that Φ_μ is locally conserved.

$$(p^\mu - p'^\mu)\Phi_\mu = -2p_k\Phi_k = 0\,.$$

This conclusion is then true for any frame of reference. Notice that formula (A3b) does not imply that $\Phi_k = 0$, since Φ_k is a complex number. With the notation

$$\Phi_k = X_k + iY_k\,,\quad X_k = \overline{X}_k\,,\quad Y_k = \overline{Y}_k\,,$$

we have

$$\mathbf{X}\perp\mathbf{Y}\perp\mathbf{p}$$

and

$$X_kX_k = Y_kY_k\,.$$

For $|h+h'|>1$ and $(p-p')^2>0$ we have $\Phi_\mu = 0$.

(iv) Case of tensor field: $\Phi_N(x) = T_{\mu\nu}(x) = \frac{1}{4}(\sigma_\mu)^{A\dot{C}}(\sigma_\nu)^{B\dot{D}}\Phi^{(1,1)}_{ABCD}$. In case of tensor fields the matrix elements for $(p-p')^2<0$ can be different from zero only if $h+h' = 0,\ \pm 1$ or ± 2. Let us concentrate upon the most interesting case $h = h' = \pm 1$. For $h = h' = 1$ we have [$\Phi_{\mu\nu}$ stands for $\Phi_{\mu\nu}(p,p',1,1)$]

$$\Phi_{00} = 0\,, \tag{A4a}$$

$$\Phi_{0k} = \Phi_{k0} = 0\,, \tag{A4b}$$

$$\Phi_{kl} = \tfrac{1}{4}(\delta^{km}\delta^{ln} - i\delta^{km}\cos\phi_r\epsilon^{rnl} - i\delta^{ln}\cos\phi_s\epsilon^{smk} - \cos\phi_s\cos\phi_r\epsilon^{smk}\epsilon^{rnl} - \cos\phi_k\cos\phi_l\cos\phi_m\cos\phi_n)\Phi_{mn}\,, \tag{A4c}$$

$$0 = (\delta^{km}\delta^{ln} + i\delta^{km}\cos\phi_r\epsilon^{rnl} + i\delta^{ln}\cos\phi_s\epsilon^{smk} - \cos\phi_s\cos\phi_r\epsilon^{smk}\epsilon^{rnl} - \cos\phi_k\cos\phi_l\cos\phi_m\cos\phi_n)\Phi_{mn}\,, \tag{A4d}$$

$$0 = (\delta^{km}\cos\phi_l\cos\phi_n + \delta^{ln}\cos\phi_k\cos\phi_m - 2\cos\phi_k\cos\phi_l\cos\phi_m\cos\phi_n)\Phi_{mn}\,, \tag{A4e}$$

$$0 = (\cos\phi_s\cos\phi_l\cos\phi_n\epsilon^{smk} + \cos\phi_r\cos\phi_k\cos\phi_m\epsilon^{rnl})\Phi_{mn}\,, \tag{A4f}$$

$$\Phi_{kl} = -(\cos\phi_k\cos\phi_l\cos\phi_m\cos\phi_n + \cos\phi_s\cos\phi_r\epsilon^{smk}\epsilon^{rnl})\Phi_{mn}\,, \tag{A4g}$$

$$\Phi_{\mu\nu} = -\Phi_{\nu\mu}$$

and if it is either self- or antiself-dual, i.e.,

$$\Phi_{\mu\nu} = \pm(i/2)\epsilon_{\mu\nu\kappa\lambda}\Phi^{\kappa\lambda}\,,$$

then

$$\Phi_{kl} = \pm i\epsilon_{klom}\Phi^{om} = 0\,.$$

Turning to an arbitrary tensor $T_{\mu\nu}$ let us subtract (A4d) from (A4c), then

$$\Phi_{kl} = -(i/2)\cos\phi_r(\epsilon^{rml}\phi_{km} + \epsilon^{rmk}\phi_{ml})\,.$$

From (A4g) follows

$$\cos\phi_k\cos\phi_l\Phi_{kl} = -\cos\phi_m\cos\phi_n\Phi_{mn} = 0\,.$$

Using this relation as well as (A4e), viz.

$$\cos\phi_l\cos\phi_n\Phi_{kn} + \cos\phi_k\cos\phi_m\Phi_{ml} = 0\,,$$

we get

$$\cos\phi_n\Phi_{kn} = \cos\phi_n\Phi_{nk} = 0\,. \tag{A5}$$

Then (A4g) yields

$$\Phi_{kl} = -\cos\phi_s\cos\phi_r\epsilon^{smk}\epsilon^{rnl}\phi_{mn}\,.$$

From that follows

$$\Phi_{kk} = 0\,. \tag{A6}$$

It is easy to see that (A5) together with (A4a) and (A4b) means

$$(p-p')^\mu\Phi_{\mu\nu} = (p-p')^\nu\Phi_{\mu\nu} = 0 \tag{A7}$$

and (A6)

$$\Phi^\mu{}_\mu = 0 \tag{A8}$$

Thus, $\Phi_{\mu\nu}$ has to be locally conserved and traceless.

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[4]See, e.g., R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964).

[5]The notation used in (1.1) is rather symbolic; what one really understands by (1.1) is a sesquilinear form

$$\lim_{R\to\infty}(\psi_{loc}, j_0(f_R f_T)\psi'_{loc})$$

extended then to an operator B; here

$$j_0(f_R f_T) = \int j_0(x)f_R(\mathbf{x})f_T(x_0,t)d^4x\,,$$

$$f_R(\mathbf{x}) = f\left(\frac{|\mathbf{x}|}{R}\right)f(x)\in\mathscr{D}(\mathbb{R}_3)\,,\quad f(x) = \begin{cases}1\,, & |s|<1\,,\\ 0\,, & |s|>2\,,\end{cases}\quad R>0\,,$$

$$f_T(x_0,t)\in\mathscr{D}(\mathbb{R}_1)\,,\quad f_T(x_0,t) = 0\quad \text{for } |x_0-t|>T\,,$$

$$\int f_T(x_0,t)dx_0 = 1\,,$$

ψ_{loc} denotes any localized state. See, e.g., C. Orzalesi, Ref. Mod. Phys. **42**, 381 (1970) and the literature quoted therein. Of course, we are assuming that the symmetry corresponding to j_0 is not spontaneously broken.

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[9]Notice that for any p with $p^2 = 0$ and $\hat{p}' = r(1,0,0,1)$, $r>0$, $(p-\hat{p}')^2 = -2r(p_0-p_3)\leqslant 0$ as $p_0\geqslant p_3$; therefore, $(p-p')^2\leqslant 0$ in any frame of reference; if $(p-p')^2 = 0$ then $p' = \lambda p$, $\lambda\geqslant 0$.

[10]This assertion can be made easily plausible for each charge B whose commutator with a certain set of field ψ is linear in these fields viz. $[B,\psi] = L(\psi)$; $L(\psi)$ linear in components of ψ. Taking into account this assumption it follows from $B\Omega = 0$ and $B\psi\Omega = 0$, where Ω and $\psi\Omega$ are the vacuum and one-particle state corresponding to the field, respectively, that $L(\psi)\Omega = 0$. This, however implies $L(\psi) = 0$. Thus B commutes with all fields of the chosen set.

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Self-gravitating fluids of class one with nonvanishing Weyl tensor

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(Received 5 January 1984; accepted for publication 26 April 1984)

All the Zeldovich fluids of imbedding class one with nonvanishing Weyl tensor have been obtained by solving equations of continuity and equations of motion. All of them are found to be irrotational and therefore can be termed as self-gravitating fluids with pressure equal to energy density.

PACS numbers: 04.20.Jb, 95.30.Sf, 98.80.Dr

I. INTRODUCTION

Barnes[1] has shown that a class one perfect fluid possesses at least one of the following properties: (i) conformal flatness, (ii) the flow is geodesic, and (iii) it admits a three-dimensional group of isometries with two-dimensional space-like trajectories. All the solutions belonging to (i) and (ii) have been obtained by Stephani[2] and Barnes.[1,3] However the solutions belonging to (iii) with nonvanishing acceleration vector (nongeodesic flow) and nonzero Weyl tensor, are quite rare. As far as the authors are aware, only one static solution of this kind is available, which has been discovered and rediscovered by many authors.[1,2,4–7] In the present article the authors have obtained all the solutions belonging to (iii) considering the barotropic equation of state, pressure equal to energy density. The possible relevance of the equation of state pressure equal to the energy density has been discussed by a number of authors[8–20] since it was first proposed by Zeldovich.[8] It is said to describe many useful situations such as radiation, relativistic degenerate Fermi gas, and ultracondensed baryon matter.[9,10] If, in addition, its motion is irrotational, then it has the same stress energy tensor as that of a zero rest mass scalar field or that of self-gravitating fluids with pressure equal to energy density.[11] Also these solutions are transformable to the solution of the Brans–Dicke theory in vacuum.[12]

II. METRIC AND CLASS ONE CONDITIONS

An appropriate metric admitting a three-parameter group of isometries with the two-dimensional trajectories $r = \text{const}$ and $t = \text{const}$ can be expressed as[1]

$$ds^2 = -A(r,t)dr^2 - B(r,t)d\sigma^2 + C(r,t)dt^2, \tag{2.1}$$

where $d\sigma^2$ is a two-dimensional metric with constant Gaussian curvature K and can be written as

$$d\sigma^2 = d\theta^2 + f^2(\theta)d\phi^2, \tag{2.2}$$

where $f(\theta) = \sin\theta, \theta, \sinh\theta$ for $K = 1, 0$, and -1, respectively. In fact these cases correspond to spherical, plane, and hyperbolic symmetries, respectively. The metric (2.1) can be transformed to five simpler metrics using the well-known transformations[21]

$$ds^2 = -A(r,t)dr^2 - r^2 d\sigma^2 + C(r,t)dt^2, \tag{2.3}$$

$$ds^2 = -A(r,t)dr^2 - r^2 d\sigma^2 + 2D(r,t)dr\,dt, \tag{2.4}$$

$$ds^2 = -A(r,t)dr^2 - t^2 d\sigma^2 + C(r,t)dt^2, \tag{2.5}$$

$$ds^2 = -t^2 d\sigma^2 + C(r,t)dt^2 + 2D(r,t)dr\,dt, \tag{2.6}$$

$$ds^2 = -A(r,t)dr^2 - h^2 d\sigma^2 + C(r,t)dt^2, \tag{2.7}$$

where h is a constant.

Now the necessary and sufficient conditions so that a metric of the type (2.1)–(2.7) may be of imbedding class one are given as[22]

$$R_{1414} = (R_{1212}R_{3434} - R_{1224}R_{1334})/R_{2323}, \tag{2.8}$$

provided $R_{2323} \neq 0$, excluding the case when "B" is merely a constant and the space-time is always of class one. The necessary part of this result is due to Geonner[23] and for spherical case ($K = 1$) due to Eiesland.[24] The conditions (2.8) can also be written in terms of the energy momentum tensor in Karmarkar's way,[25] e.g.,

$$3F^2 + 8\pi F(4T_2^2 - T_1^1 - T_4^4) + 64\pi^2(T_1^4T_4^1 - T_1^1T_4^4) = 0, \tag{2.9}$$

where

$$F = -R_{2323}/B^2 f^2(\theta). \tag{2.10}$$

Further the Einstein field equations for perfect fluid distribution are given by

$$R_j^i - \tfrac{1}{2}R\delta_j^i = -(a+b)v^i v_j + b\delta_j^i = -8\pi T_j^i, \tag{2.11}$$

a and b being 8π times the energy density and pressure, respectively. Here v^i stands for the mean dynamical velocity vector, i.e., the flow vector.

Now in view of (2.11), the condition (2.9) leads to

$$(3F - a)(F - b) = 0. \tag{2.12}$$

The vanishing of the first factor gives a space-time with vanishing Weyl tensor, while the second factor when equated to zero gives a space-time with nonvanishing Weyl tensor. In the next section, the Zeldovich fluids for the later case, i.e.,

$$F = b, \tag{2.13}$$

will be determined by considering the alternative metrics (2.3)–(2.7).

III. CLASS ONE ZELDOVICH FLUIDS WITH NONZERO WEYL TENSOR

Because of (2.11), T_j^i satisfies a conservation equation of the type

$$T_{j;i}^i = 0, \tag{3.1}$$

where a semicolon indicates the covariant derivative. For the

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perfect fluid case (2.11), (3.1) leads to the equation of continuity

$$a_i v^i + (a+b)\Phi = 0, \tag{3.2}$$

and to the equation of motion

$$b_{,i} v^i v_k + (a+b)\dot{v}_k - b_{,k} = 0, \tag{3.3}$$

where Φ $(= v^i_{;i})$ and $\dot{v}_k$ $(= v_{k;i}v^i)$ are the volume expansion and the acceleration vector, respectively, and where a comma and a semicolon denote the ordinary and covariant derivatives, respectively.

Case (*A*): The equations (3.2) and (3.3) with reference to the metric (2.3) and using Eq. (2.13) give rise, for $a = b$, to

$$\frac{b^{\cdot\prime}}{b^{\cdot}} - \frac{rb'' + 3b'}{rb' + 2b} = 0, \tag{3.4}$$

$$\frac{2b^{\cdot\prime}}{b^{\cdot}} - \frac{r(2b'r + 6b)}{(4b + b'r)(b'r + 2b)}b'' - \frac{2br}{K - br^2} - \frac{5b'}{4b + b'r} - \frac{3b'}{b'r + 2b} + \frac{2}{r} = 0 \tag{3.5}$$

provided $b^{\cdot} \neq 0$. The prime and dot indicate partial derivatives with respect to "r" and "t," respectively. The expressions for unknown metric potentials, flow vectors, and vorticity ω_{ab} are given as

$$\begin{aligned} A &= (K - br^2)^{-1}, \\ C &= b^{\cdot 2}r^2[(K - br^2)(b'r + 2b)(b'r + 4b)]^{-1}, \\ v^1 &= -[(b'r + 2b)(K - br^2)/2b]^{1/2}, \\ v^4 &= \left[\frac{b'r + 4b}{b^{\cdot}r}\right]\left[\frac{(K - br^2)(b'r + 2b)}{2b}\right]^{1/2}, \end{aligned} \tag{3.6}$$

$v^2 = v^3 = 0$, and $\omega_{ab} = 0$ (hence implies irrotational flow).

Equation (3.4) is easily integrable and gives

$$b = \phi(u)/r^2, \tag{3.7}$$

where $u = r^{\cdot}\, G(t)$, $G(t)$ being an arbitrary function. Also ϕ of (3.7) is further restricted by (3.5) as follows:

$$[u\bar{\phi} + 2\phi][K - \phi] = \alpha = 2C + K^2/2 \quad \text{(let)}, \tag{3.8}$$

where α and C are aribtrary constants and $\bar{\phi} \equiv d\phi/du$.

Equation (3.8) gives on integration the following expression:

$$\log pu^4(\phi^2 - K\phi + \alpha/2) = \begin{cases} \dfrac{K}{\sqrt{C}} \tan^{-1} \dfrac{\phi - K/2}{\sqrt{C}}, & \text{for } C > 0, \\ \dfrac{K}{2\sqrt{-C}} \log \dfrac{\phi - K/2 - \sqrt{-C}}{\phi - K/2 + \sqrt{-C}}, & \text{for } C < 0, \\ -\dfrac{K}{\phi - K/2}, & \text{for } C = 0. \end{cases} \tag{3.9}$$

Owing to (3.7) and (3.8), the contents of (3.6) can be expressed in terms of ϕ in a more informative form:

$$\begin{aligned} A &= (K - \phi)^{-1}, \quad C = \frac{r^2\dot{G}^2}{\alpha G^2}[\alpha(K - \phi)^{-1} - 2\phi], \quad \alpha > 0, \\ v^1 &= -\left[\frac{\alpha - 2\phi(K - \phi)}{2\phi}\right]^{1/2}, \\ v^4 &= -\frac{\alpha G}{r\dot{G}}[\alpha - 2\phi(K - \phi)]^{-1}v^1, \\ v^2 &= v^3 = 0. \end{aligned} \tag{3.10}$$

As is clear from (3.9), ϕ is occurring implicity and therefore the study of the fluid distributions (in general) is not that straightforward. However some conclusion can still be drawn, e.g., solutions in plane symmetry ($K = 0$) and hyperbolic symmetry ($K = -1$) are not valid in the present case as the signature of the metric is disturbed. The signature could have been preserved provided $\phi < 0$. But this implies negative pressure (or energy density), which violates the energy condition

$$T_{ij}v^iv^j \geqslant 0$$

and the Hawking–Penrose conditions[26]

$$[T_{ij} - \tfrac{1}{2}g_{ij}T]v^iv^j \geqslant 0. \tag{3.11}$$

The conditions (3.11) require positiveness of pressure (or energy density) for the present equation of state. The case with vanishing ϕ simply imply the flat space as Szekers[27] has shown that there are no class one vacuum space-times. So the only valid solutions associated with the metric (2.3) are spherically symmetric. Some explicit solutions of this type can be obtained by considering $C = -\frac{1}{16}, -\frac{1}{36}, -\frac{1}{64}, -1$ and then solving quadratic, cubic, and biquadratic equations in ϕ so obtained from the second of (3.9). The equations (3.4) and (3.5) are not valid for $b^{\cdot} = 0$. Therefore recalculations with $A = A(r)$ give rise the following data as an alternative to (3.10):

$$\begin{aligned} &A = 2/K, \qquad C = r^2, \\ &v_1 = v_2 = v_3 = 0, \qquad v_4 = \mp r, \\ &b = K/2r^2, \qquad K = 1, \end{aligned}$$

and nonvanishing acceleration components are given by

$$\dot{v}_1 = -1/r, \quad \dot{v}_4 = 0.$$

The volume expansion ϕ and shear σ_{ab} are zero.

Case (*B*): The equation of continuity (3.2) and the equation of motion (3.3) for the metric (2.5), taking (2.13) into account for $a = b$, can be expressed as

$$\frac{b^{\cdot\prime}}{b'} - \frac{3b^{\cdot} + b^{\cdot\cdot}t}{2b + b^{\cdot}t} = 0, \tag{3.12}$$

$$\frac{2b'}{b'} - \frac{t(2b^{\cdot}t + 6b)}{(4b + b^{\cdot}t)(b't + 2b)}b^{\cdot\cdot} + \frac{2bt}{bt^2 - K} - \frac{5b^{\cdot}}{4b + b^{\cdot}t} - \frac{3b^{\cdot}}{b^{\cdot}t + 2b} + \frac{2}{t} = 0, \tag{3.13}$$

provided $b' \neq 0$. We observe that (3.12) and (3.13) are exactly parallel to (3.4) and (3.5). The rest of the work for this case, can be carried out on the same footings as that of preceding case and we come across the following essential data:

$$\begin{aligned} &C = (\phi - K)^{-1}, \quad A = \frac{t^2F'^2}{\beta F^2}[\beta(\phi - K)^{-1} + 2\phi], \quad \beta > 0, \\ &v^1 = -(\beta F/tF')[\beta + 2\phi(\phi - K)]^{-1}v^4, \\ &v^4 = \left[\frac{\beta + 2\phi(\phi - K)}{2\phi}\right]^{1/2}, \quad \omega_{ab} = 0. \\ &b = \phi(u)/t^2, \quad u = tF(r), \\ &F(r) \text{ is an arbitrary function,} \end{aligned} \tag{3.14}$$

where ϕ is given by

$$[u\dot{\phi} + 2\phi][\phi - K] = -\beta, \quad \beta > 0. \tag{3.15}$$

Solution of (3.15) is exactly similar to those in (3.9). Contrary to case (A), the present case may have valid solutions corresponding to $K = 0$ (plane symmetric) and $K = -1$ (hyperbolic) along with the spherically symmetric case ($K = 1$). Particular explicit solutions corresponding to $K = \pm 1$ can be obtained by supposing the same values of the arbitrary constant as in case (A) (with $\pm$ sign). However for the plane symmetric case all the solutions can be obtained explicitly by putting $K = 0$ in the second solution of the analogous set and we get

$$b = \sqrt{(q^2/t^4F^4 - \beta/2)}, \quad \text{const } q > 0.$$

The continuity equation (3.12) and the equation of motion (3.13) become meaningless for $b' = 0$. So fresh calculations with $C = C(t)$ give

$$A = 1, \quad C = (\alpha^2/t^2 - K)^{-1},$$
$$v_1 = v_2 = v_3 = 0, \quad v_4 = \mp(\alpha^2/t^2 - K)^{-1/2},$$
$$b = \alpha^2/t^4, \quad K = 1, 0, -1.$$

Also the volume expansion ϕ, acceleration $\dot{v}_i$, and shear σ_{ab} are given as

$$\phi = (2/t)\sqrt{(\alpha^2/t^2 - K)}$$
$$\dot{v}_i = (0,0,0,0), \quad \sigma_{22} = \frac{\sigma_{33}}{f^2} = -\frac{t}{3}\left[\frac{\sigma^2}{t^2} - K\right]^{1/2}.$$

The rest of the shear components are zero.

The metric in this case admits a four parameter group of isometries with the trajectories $t = \text{const}$ (see Ref. 1). The metric representing the above solution can be transformed by Tabensky form (for $K = 0$) (see Ref. 11) as

$$ds^2 = (1/4\alpha^2)(dT^2 - dR^2) - T\,d\sigma^2, \quad T = t^2 \text{ and } R = 2\alpha r.$$

Letelier[15] has shown that the above metric has singularity at $T = 0$ of semi-Kasner class.

ACKNOWLEDGMENT

The authors are indebted to Professor S. N. Pandey for suggesting the problem of perfect fluids of class one with nonvanishing Weyl conformal curvature tensor and would like to thank him for much helpful advice during the preparation of the aritcle.

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Constraints on the nature of inertial motion arising from the universality of free fall and the conformal causal structure of space-time

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(Received 27 March 1984; accepted for publication 15 June 1984)

According to the principle of the universality of free fall, the motions of all neutral monopole particles are governed by one common path structure. This principle does not, however, require the path structure to be geodesic; that is, the path structure need not be a projective structure. It is shown that any equation of motion structure (either a curve or a path structure) that has sufficient microisotropy to be compatible with the conformal causal structure of space-time must be geodesic and must be unique. Hence, the empirically well-supported principles of conformal causality and of the universality of free fall together require the existence of a unique Weyl structure on space-time.

PACS numbers: 04.20.Me, 04.20.Cv, 02.40.Ky

I. INTRODUCTION

The transition from the kinematic to the dynamic analysis of the motions of bodies in space-time theories has traditionally been viewed to consist in the determination of a particular class of *standard motions* that are the *free motions*. The concept of force is then defined in terms of acceleration relative to the standard of *no-acceleration* provided by these free motions. This procedure is meaningful if and only if for each event of space-time and for every timelike direction at that event, there exists one and only one standard motion through that event. From a geometric viewpoint, the determination of the class of standard motions amounts to the determination of a *path* structure for the space-time manifold.

The problem of motion[1] concerns the nature of this transition. The controversy surrounding this problem has nurtured and given currency to a number of claims concerning the status and meaning of the laws of inertia of the various space-time theories: the laws (1) are conventional in character, (2) are definitions, (3) are circular and without empirical content, and (4) postulate the existence of free particles or of inertial reference frames.

Those who argue for the conventional and/or definitional character of the laws mainly on *epistemic* grounds point out that the laws do not supply *independent* criteria of what is to count as *force-free or natural motion*. The only way of knowing when no forces act on a body is that it moves as a free particle along the geodesics of space-time. But how, without already knowing the geodesics (or the projective structure) of space-time, is it possible to determine which particles are free and which are not? And of course, to determine the projective structure of space-time it is necessary to use free particles. The circularity, they argue, cannot be avoided.

Others have tried to define a *free particle* with respect to an *inertial frame* as a particle the motions of which satisfy the equation $d^2x^\alpha/dt^2 = 0$ in that frame. But how is one to determine what an inertial frame is? If an inertial frame is to be characterized as a frame in which the motion of a free particle would satisfy the equation $d^2x^\alpha/dt^2 = 0$, then the definition is obviously circular. Hence, Newton's first law is interpreted by some as the *existence* claim: there exist physical inertial frames in which the motions of free particles would be governed by the equation $d^2x^\alpha/dt^2 = 0$. There remains, however, the lack of noncircular physical criteria for identifying these frames.

Those who argue for the conventional character of the laws of inertia from *ontological* considerations concerning the nature of space-time structure and/or for their *relationalist* character from a Leibnizian–Machian view of motion (the view according to which relative motion must be understood as relative motion of bodies with respect to each other or with respect to material reference frames) advance the thesis that what counts as a standard of no-acceleration or free motion is *not* dictated by a physically real and causally efficacious inertial structure of space-time.

In addition to its importance for the foundations of mechanics, the problem concerning free or natural motion has recently become a pressing issue within the particular context of the constructive axiomatics for the general theory of relativity (GTR). One of the constructive axioms employed by Ehlers, Pirani, and Schild,[2] the projective axiom, is a statement of the infinitesimal version of the law of inertia, the law of free (fall) motion which contains Newton's first law of motion as a special case in the absence of gravitation. The problem is how to introduce a class of preferred motions, that is, how to characterize that particular path structure that would govern the motions of free particles (neutral, spherically symmetric nonrotating test bodies) while avoiding the circularity problem surrounding the notion of a free particle.[3]

In previous work,[4,5] we have solved these difficulties. Our solution provides noncircular, empirical procedures for the identification of monopoles, for the separation of monopole particles into distinct classes each of which corresponds to a particular path structure, for the measurement of these

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path structures, and for the testing of a given path structure for geodesicity. We have also appropriately reformulated the laws of motion. This reformation is also briefly indicated below in Sec. II.

In this paper, we prove that in a world in which causal relations are determined by a conformal structure, the only possible solution to the problem of motion is the solution we have given; that is, the standard, free motions are determined by a physically real projective structure and this projective structure must be unique.

The nature and significance of the results of this paper are discussed in detail in Sec. II. Section III is devoted to a discussion of curve and path structures in general, of the relationship between them, and of the condition that any such field that governs the motions of *neutral* monopoles must satisfy to be compatible with the special theory of relativity (STR). In Sec. IV, it is proved that any curve structure that satisfies this compatibility condition must be geodesic. In Sec. V, the corresponding result for path structures is proved. Finally, in Sec. VI, it is proved that unless the projective structure of space-time is unique, there exists a subspace structure in some region of space-time.

II. IMPLICATIONS FOR GEOMETRIC REALISM

In this section, we discuss the implications that the theorems proved below have for the foundations of the general theory of relativity (GTR).

First, consider a world without fields, a space-time equipped with only a differential structure. In such a world, it is possible to define curves and paths (unparametrized curves) and their elements. However, there are no preferred curves or paths, and the motion of material bodies is not predictable. The simplest type of particles are monopole or unstructured particles. Experience indicates that the (four- or three-) acceleration of a massive body cannot be freely chosen. In particular, a monopole particle is characterized by the fact that at any event on its world line, its (four- or three-) velocity at that event is sufficient to determine its (four- or three-) acceleration at that event. That there must exist additional, postdifferential structure to account for this phenomenon is evident from the inhomogeneous nature of the transformation laws for four-acceleration (3.3) and for three-acceleration (3.4). We are led to the following principle.

The predictability of motion (*PM*): Corresponding to every type of massive monopole, there exists either an acceleration field or a directing field which governs the motion of that type of particle. Directing fields correspond to a special subclass of acceleration fields. The specific relationship is detailed below in Sec. III E.

It is evident that many different acceleration fields might exist and that the set of actually existing acceleration (or directing) fields need not exhibit any pattern of relationships. However, the well-known example of the set of directing fields that govern the motions of monopoles which have various electromagnetic charge to mass ratios suggests that the contrary is the case. The notion of charge-to-mass ratios may be characterized in the following way.[6]

Definition of charge to mass ratios: Suppose that the acceleration fields that are known to exist on space-time constitute a parametrized family of the form

$$A^{\,i}_{\,2}(x^i,\gamma^i_1) = U^{\,i}(x^i,\gamma^i_1) + \sum_a \lambda_a K^{\,i}_{\,a}(x^i,\gamma^i_1)\,, \tag{2.1}$$

where U is a specific acceleration field, the K_a are four-force fields, and the λ_a are scalars that are independent of the variables x^i and γ^i_1. The parameters λ_a are called charge-to-mass ratios. In case every acceleration field in the family corresponds to a directing field, the directing fields form a parameterized family of the form

$$\Xi^{\alpha}_{\,2}(x^i,\xi^{\,\alpha}_1) = W^{\alpha}(x^i,\xi^{\,\alpha}_1) + \sum_a \lambda_a\, F^{\alpha}_{\,a}(x^i,\xi^{\,\alpha}_1)\,, \tag{2.2}$$

where W is the directing field and the F_a are three-force fields corresponding to the fields U and K_a. The acceleration field U (or the directing field W) determines the common zero for the charge-to-mass parameters λ_a and governs the motions of *neutral* monopoles. Note that by definition, short-range forces are essentially zero except in a very small region surrounding a source; consequently, only charges, such as the electromagnetic charge, which couple to long-range forces are of interest in the present context.

A microsymmetry[7] of an acceleration field or of a directing field at an event p is a local diffeomorphism of a neighborhood of p which leaves p fixed and preserves the field at the event p. The set of microsymmetries at p forms the microsymmetry group at p. If the motions of monopoles are to be in accord with the principles of STR then at every event p of space-time, the field that governs the motions of neutral monopoles must be micro-Lorentz invariant and the force fields that couple to the various charges must be micro-Lorentz covariant. Thus at each event p, the first-order part of the microsymmetry group of the field governing the motions of neutral monopoles must contain a subgroup that is isomorphic to the Lorentz group. The theorems presented in Sec. IV establish that any acceleration field that satisfies this condition of compatibility with STR must be geodesic. The corresponding theorems for directing fields are presented in Sec. V.

An example of a one-parameter family of acceleration fields which does not correspond to a one-parameter family of directing fields is given by

$$A^{\,i}_{\,2}(x^i,\gamma^i_1) = -\Gamma^{\,i}_{jk}(x^i)\gamma^j_1\gamma^k_1 + \lambda F^{\,i}_{\,j}(x^i)\gamma^j_1\,. \tag{2.3}$$

This family should be contrasted with the family (3.22) which corresponds to the directing field family (3.23). The acceleration field (2.3) gives rise to a directing field only for $\lambda = 0$. However, all acceleration fields that are presently known correspond to directing fields. Moreover, the three-acceleration at a given event for a given three-velocity is the same for all neutral monopoles regardless of mass and regardless of material composition. Since the only long-range charge known to exist is the electromagnetic charge, these observations can be formulated as follows.

The universality of free fall (*UFF*): The set of all actually existing equation-of-motion structures for massive monopoles constitutes a one-parameter family of directing fields of the form

$$\Xi^{\alpha}_{2}(x^i,\xi^{\alpha}_{1}) = W^{\alpha}(x^i,\xi^{\alpha}_{1}) + (Q/m)\,F^{\alpha}(x^i,\xi^{\alpha}_{1})\,, \tag{2.4}$$

where W is a specific directing field and Q/m is the electromagnetic charge-to-mass ratio. Since this principle asserts that gravitational charges do *not* exist, it has been called the principle of equivalence of gravitational and inertial mass or the weak principle of equivalence. However, the weak principle of equivalence is frequently construed to require not only the uniqueness of the directing field W which governs the motions of neutral monopoles but also its geodesicity.[8] This much stronger statement is formulated as the following principle.

The geodesicity of free fall (*GFF*): The directing field W that governs the motions of all neutral monopoles is geodesic. The principle UFF and the compatibility of the directing field W with STR jointly entail by the theorems of Sec. V the principle GFF.

In our previous work, we have shown that directing fields can be measured given only access to the differential structure of space-time, that is, given only the ability to set up local coordinate systems and to track material bodies with respect to such coordinate systems. In contrast, acceleration fields can only be measured by much more complicated and indirect means that require the prior measurement of other geometric structure fields.[9] The direct measurability of directing fields and the principles UFF and GFF account for the fact that directing fields play a much more prominent role in the foundations of GTR than acceleration fields. For this reason, separate proofs have been provided in Sec. V for the theorems concerning directing fields even though it is possible from a purely mathematical viewpoint to rearrange the exposition so that these results follow as corollaries of the corresponding theorems for acceleration fields presented in Sec. IV.

The principles UFF and GFF are empirically testable given access only to the differential structure of space-time because directing fields can be measured at least in principle on that basis alone. The principle UFF is falsified if two independent differences of three distinct directing fields are not constant multiples of each other. The principle GFF is falsified unless for every directing field $\Xi^{\alpha}_{2}(x^i,\xi^{\alpha}_{1})$ there exists some constant multiple of the difference field $k\,(\Xi^{\alpha}_{A2}(x^i,\xi^{\alpha}_{1}) - \Xi^{\alpha}_{B2}(x^i,\xi^{\alpha}_{1}))$ such that

$$\Xi^{\alpha}_{2}(x^i,\xi^{\alpha}_{1}) + k\,(\Xi^{\alpha}_{A2}(x^i,\xi^{\alpha}_{1}) - \Xi^{\alpha}_{B2}(x^i,\xi^{\alpha}_{1})) \tag{2.5}$$

is geodesic. Note that a directing field can be tested for geodesicity simply by computing derivatives with respect to the variables ξ^{α}_{1}. Such direct and elementary tests are difficult to perform and consequently have not yet been carried out. However, the principle UFF has been tested to very high precision by indirect experiments of the Eötvösz type.[10] Also, given the theorems proved in this paper, the various experimental tests of STR are indirect tests of the principle GFF.

Consider a world equipped with a two-parameter family of acceleration fields of the form

$$\begin{aligned} A^{i}_{2}(x^i,\gamma^i_1) = &-\Gamma^{i}_{jk}(x^i)\gamma^j_1\gamma^k_1 + \lambda S^{i}_{jk}(x^i)\gamma^j_1\gamma^k_1 \\ &+ (Q/m)(g_{rs}(x^i)\gamma^r_1\gamma^s_1)^{1/2}F^{i}_{j}(x^i)\gamma^j_1\,, \end{aligned} \tag{2.6}$$

where $S^{i}_{jk}(x^i)$ is a tensor field. The parameter might, for example, be a gravitational charge-to-mass ratio. All of the fields with zero electromagnetic charge-to-mass ratio are geodesic. There is no reason to identify any one of them as the field which governs free fall; that is, there is no unique zero for the parameter λ. However, in Sec. VI, it is shown that such a state of affairs is in conflict with STR. First, any geodesic directing field (or projective structure) must satisfy a second-order condition of compatibility with the conformal causal structure of space-time for otherwise the material bodies governed by the directing field can break the light barrier. Moreover, if two projective structures exist in a region of space-time which differ throughout that region, then a nonvanishing covector field, and hence a subspace structure, is defined throughout the region. Consequently, the projective structure of space-time must be unique, and hence there exists a unique Weyl structure on space-time determined by the conformal and projective structures of space-time.[11]

In summary, the empirically well-supported principle UFF asserts the existence of a unique directing field which governs the motions of neutral monopoles. The requirement that this field possess a sufficient degree of microisotropy to be compatible with STR forces this field to be geodesic. The requirement that massive bodies not break the light barrier ensures that this projective structure is compatible with the conformal causal structure of space-time and that these structures determine a Weyl structure. The additional requirement that no subspace structure exist in any region of space-time entails the uniqueness of the projective structure and hence of the Weyl structure. Furthermore, it is *not* possible to avoid the requirement of geodesicity of free motion by appealing to more general types of acceleration fields that do not give rise to directing fields.

These results motivate the following reformulation of Newton's laws of motion which we have discussed at length elsewhere.[12]

The law of inertia: There exists on space-time a unique projective structure Π (or equivalently, a unique geodesic directing field Π). Free motion is defined with reference to the projective structure Π as follows.

Definition of free motion: A possible or actual material body is in a state of free motion during any part of its history just in case the corresponding segment of its world line path is a solution path of the differential equation determined by the unique projective structure of space-time. The law of inertia and the definition of free motion together constitute a modern reformulation of Newton's first law of motion. Newton's second law of motion may be reformulated as follows.

The law of motion: With respect to any coordinate system, the world line path of a possible or actual material body satisfies an equation of the form

$$m(\xi^{\alpha}_{2} - \Pi^{\alpha}_{2}(x^i,\xi^{\alpha}_{1})) = F^{\alpha}(x^i,\xi^{\alpha}_{1})\,, \tag{2.7}$$

where m is a scalar constant characteristic of the material body called its inertial mass and $F^{\alpha}(x^i,\xi^{\alpha}_{1})$ is the three-force acting on the body. Note that the law of motion makes explicit use of the unique projective structure Π on space-time. The law of motion, therefore, depends ontologically on the law of inertia; consequently, it is impossible to derive the law of inertia from the law of motion.

It was pointed out in the Introduction that the long-standing difficulties surrounding the law of inertia led many authors to reject the physical reality of at least certain aspects of the geometry of space-time, most notably the projective structure of space-time. It is clear from the above discussion and from the analysis of directing field structures presented in our previous work that such a position is now untenable. Our results compel the adoption of a realist field ontology of the geometric structures of space-time. Weyl was an early and forceful proponent of this viewpoint. To emphasize the necessity for a physically real and causally efficacious inertial structure of space-time, a structure he called the guiding field, he devised the following paradox[13]:

> Incidentally, without a world structure the concept of relative motion of several bodies has, as the postulate of general relativity shows, no more foundation than the concept of absolute motion of a single body. Let us imagine the four-dimensional world as a mass of plasticine traversed by individual fibers, the world lines of material particles. Except for the condition that no two world lines intersect, their pattern may be arbitrarily given. The plasticine can then be continuously deformed so that not only one but all fibers become vertical straight lines. Thus no solution of the problem is possible as long as in adherence to the tendencies of Huyghens and Mach one disregards the structure of the world. But once the inertial structure of the world is accepted as the cause for the dynamical inequivalence of motions, we recognize clearly why the situation appeared so unsatisfactory. ...Hence the solution is attained as soon as we dare to acknowledge the inertial structure as a real thing that not only exerts effects upon matter but in turn suffers such effects.

Let us analyze this example using the concept of the microsymmetry group of a geometric structure at an event p. Consider a space-time manifold equipped only with a differentiable structure, the plasticine of Weyl's example. Then all diffeomorphisms preserve this structure; consequently, the microsymmetry group at any event p is an infinite-parameter group isomorphic to the group of all invertible formal power series in four variables. Clearly, given an infinite number of parameters, one can straighten out an arbitrary pattern of world lines (fibers) in the neighborhood of any event. In contrast, the active microsymmetry group of a projective structure at any event of space-time is a 20-parameter Lie group isomorphic to the group P_n^2 (see Theorem 5.3). The fact that only a finite number of parameters are available prevents an arbitrary realignment of the world lines of material bodies in the neighborhood of any given event.

Weyl's plasticine example shows that the Leibnizian view of relative motion, namely the view according to which all motion must be defined as motion relative to bodies, is self-defeating in GTR. The fact that a stationary, homogeneous elastic sphere will, when set in rotation, bulge at the equator and flatten at the poles is well known. According to Weyl, this phenomenon is to be accounted for in the following way. The complete physical system consisting of both the body and the local inertial-gravitational field is not the same in the two situations. The cause of the effect is the state of motion of the body with respect to the local gravitational field and is not, indeed as Weyl's plasticine example shows cannot, be the state of motion of the body relative to other bodies. To attribute the effect as Einstein[14] and Mach did to the rotation of the body with respect to the other *bodies* in the universe is to endorse a remnant of the unjustified monopoly of the older body ontology, namely, the sovereign right of material bodies to play the role of physically real and acceptable causal agents.

III. THE GEOMETRY OF THE INERTIAL STRUCTURE

Denote by M the n-dimensional, C^∞ manifold which represents space-time. A curve in M is a map $\gamma: \mathbb{R}\to M$ and a path in M is an equivalence class $\xi = [\gamma]$ of such maps any two of which are related by an invertible parameter transformation $\mu: \mathbb{R}\to\mathbb{R}$. For convenience, in the discussion of curve and path elements at some particular point $p\in M$, attention is restricted to those curves which satisfy $\gamma(0) = p$ and to those parameter transformations which satisfy $\mu(0) = 0$.

A. Curve and path elements

A *curve element* [15] of order k at $p\in M$ is an equivalence class $j_0^k\gamma$ of curves through p which have the same Taylor expansion with respect to some (and hence every) coordinate chart $(U,x)_p$ up to and including order k at $0\in\mathbb{R}$. A *path element* of order k at $p\in M$ is an equivalence class of paths $j_p^k\xi$ consisting of all paths corresponding to curves in $j_0^k\gamma$, where $\gamma\in\xi$.

A second-order curve element $j_0^2\gamma$ has local coordinates γ_1^i and γ_2^i called n-velocity and n-acceleration, respectively, and given by

$$\gamma_1^i = \frac{d}{d\lambda}x^i\circ\gamma(0)\,,\quad \gamma_2^i = \frac{d^2}{d\lambda^2}x^i\circ\gamma(0)\,. \tag{3.1}$$

A second-order path element $j_p^2\xi$ has local coordinates ξ_1^α and ξ_2^α called $(n-1)$-velocity and $(n-1)$-acceleration, respectively, and given by

$$\xi_1^\alpha = \left.\frac{dx^\alpha\circ\gamma}{dx^n\circ\gamma}\right|_p\,,\quad \xi_2^\alpha = \left.\frac{d^2x^\alpha\circ\gamma}{(dx^n\circ\gamma)^2}\right|_p\,. \tag{3.2}$$

Under a change of coordinate chart from $(U,x)_p$ to $(\bar U,\bar x)_p$, the coordinates of $j_0^2\gamma$ transform according to

$$\bar\gamma_1^i = \bar X_j^i\gamma_1^j\,,\quad \bar\gamma_2^i = \bar X_j^i\gamma_2^j + \bar X_{jk}^i\gamma_1^j\gamma_1^k\,, \tag{3.3}$$

and the coordinates of $j_p^2\xi$ transform according to

$$\begin{aligned}\bar\xi_1^\alpha &= (\bar X_n^\alpha + \bar X_{\beta}^{\alpha}\xi_1^\beta)/(\bar X_n^n + \bar X_\gamma^n\xi_1^\gamma)\,,\\ \bar\xi_2^\alpha &= (\bar X_\rho^\alpha\xi_2^\rho + \bar X_{\rho\sigma}^\alpha\xi_1^\rho\xi_1^\sigma + 2\bar X_{n\rho}^\alpha\xi_1^\rho + \bar X_{nn}^\alpha)/\\ &\quad\cdot(\bar X_n^n + \bar X_\gamma^n\xi_1^\gamma)^2\,,\\ &\quad -\bar\xi_1^\alpha(\bar X_\rho^n\xi_2^\rho + \bar X_{\rho\sigma}^n\xi_1^\rho\xi_1^\sigma + 2\bar X_{n\rho}^n\xi_1^\rho + \bar X_{nn}^n)/\\ &\quad(\bar X_n^n + \bar X_\gamma^n\xi_1^\gamma)^2\,,\end{aligned} \tag{3.4}$$

where $\bar X = \bar x\circ x^{-1}$.

B. The role of the inertial structure

Although the transformation laws for γ_2^i and ξ_2^α are both linear, they are *not* homogeneous in the acceleration variables. Thus there does not exist a unique standard of zero

acceleration that is intrinsic to the differential topological structure of space-time. Moreover, even the difference of the accelerations of two bodies at the same space-time point has no absolute meaning unless their velocities happen to be the same. Hence, additional structure in the form of a geometric structure field called the inertial structure of space-time or the guiding field is required to provide the unique standard of zero acceleration. This field may be either an acceleration field or a directing field.

C. Acceleration and directing fields

Denote by $\mathscr{L}^1_1(M)$ and $\mathscr{L}^2_1(M)$ the bundles of first- and second-order curve elements and by $\mathscr{D}^1(M)$ and $\mathscr{D}^2(M)$ the bundles of first- and second-order path elements. In each case, the bundle of second-order elements can be regarded as a bundle over the corresponding bundle of first-order elements.

An acceleration field[16] is a cross section A: $L^1_1(M)\to L^2_1(M)$. Such a field is described in terms of local coordinates by functions $A^i_2(x^i,\gamma^i_1)$ which transform under a change of coordinate chart according to

$$\overline{A}^i_2(\bar{x}^i,\bar{\gamma}^i_1)=\overline{X}^i_j(x^i)A^j_2(x^i,\gamma^i_1)+\overline{X}^i_{jk}(x^i)\gamma^j_1\gamma^k_1\,. \tag{3.5}$$

If $j^2_0\gamma$ is a curve element at p with first-order part $j^1_0\gamma$, then $\gamma^i_2-A^i_2(x^i,\gamma^i_1)$ transforms both linearly *and* homogeneously; consequently, there exists a coordinate independent zero for these relative n-accelerations. An acceleration field is called geodesic iff for every $p\in M$, there is some chart, $(\overline{U},\bar{x})_p$, such that the functions $\overline{A}^i_2(\bar{x}^i,\bar{\gamma}^i_1)$ vanish at p. A geodesic acceleration field (affine structure) is denoted by Γ and has the special functional form

$$\Gamma^i_2(x^i,\gamma^i_1)=-\Gamma^i_{jk}(x^i)\gamma^j_1\gamma^k_1\,. \tag{3.6}$$

An acceleration field A determines a curve structure on M by means of the differential equation

$$\frac{d^2x^i\circ\gamma}{d\lambda^2}=A^i_2\left(x^i\circ\gamma,\frac{dx^i\circ\gamma}{d\lambda}\right). \tag{3.7}$$

A directing field is a cross section $\Xi:\mathbb{D}^1(M)-\mathbb{D}^2(M)$. Such a field is described in terms of local coordinates by functions $\Xi^\alpha_2(x^i,\xi^\alpha_1)$ which transform under a change of coordinate chart according to

$$\begin{aligned}\Xi^\alpha_2(\bar{x}^i,\bar{\xi}^\alpha_1)=&\frac{\overline{X}^\alpha_\rho(x^i)\Xi^\rho_2(x^i,\xi^\alpha_1)+\overline{X}^\alpha_{\rho\sigma}(x^i)\xi^\rho_1\xi^\sigma_1+2\overline{X}^\alpha_{n\rho}(x^i)\xi^\rho_1+\overline{X}^\alpha_{nn}(x^i)}{(\overline{X}^n_n(x^i)+\overline{X}^n_\gamma(x^i)\xi^\gamma_1)^2}\\&-\bar{\xi}^\alpha_1\frac{\overline{X}^n_\rho(x^i)\Xi^\rho_2(x^i,\xi^\alpha_1)+\overline{X}^n_{\rho\sigma}(x^i)\xi^\rho_1\xi^\sigma_1+2\overline{X}^n_{n\rho}(x^i)\xi^\rho_1+\overline{X}^n_{nn}(x^i)}{(\overline{X}^n_n(x^i)+\overline{X}^n_\gamma(x^i)\xi^\gamma_1)^2}\,.\end{aligned} \tag{3.8}$$

For a path element $j^2_p\xi$ with first-order part $j^1_p\xi$, the relative $(n-1)$-acceleration $\xi^\alpha_2-\Xi^\alpha_2(x^i,\xi^\alpha_1)$ transforms both linearly *and* homogeneously; consequently, the zero for these relative $(n-1)$-accelerations is coordinate independent. A directing field is called geodesic iff for every $p\in M$, there is some chart $(\overline{U},\bar{x})_p$, such that the functions $\Xi^\alpha_2(\bar{x}^i,\bar{\xi}^\alpha_1)$ vanish at p. A geodesic directing field (projective structure) is denoted by Π and has the special functional form

$$\begin{aligned}\Pi^\alpha_2(x^i,\xi^\alpha_1)=&\xi^\alpha_1(\Pi^n_{\rho\sigma}(x^i)\xi^\rho_1\xi^\sigma_1+2\Pi^n_{n\rho}(x^i)\xi^\rho_1+\Pi^n_{nn}(x^i))\\&-(\Pi^\alpha_{\rho\sigma}(x^i)\xi^\rho_1\xi^\sigma_1+2\Pi^\alpha_{n\rho}(x^i)\xi^\rho_1+\Pi^\alpha_{nn}(x^i))\,,\end{aligned} \tag{3.9}$$

where the projective coefficients $\Pi^i_{jk}(x^i)$ are traceless so that $\Pi^n_{nn}(x^i)$ and $\Pi^n_{n\rho}(x^i)$ may be eliminated from (3.9). A directing field Ξ determines a path structure on M by means of the differential equation

$$\frac{d^2x^\alpha\circ\gamma}{(dx^n\circ\gamma)^2}=\Xi^\alpha_2\left(x^i\circ\gamma,\frac{dx^\alpha\circ\gamma}{dx^n\circ\gamma}\right). \tag{3.10}$$

D. The inertial structure and free fall

Either of the differential equations (3.7) and (3.10) can account for a kind of free-fall motion because it is always possible to choose a coordinate system, say $(\overline{U},\bar{x})_p$, in which the fields $\overline{A}^i_2(\bar{x}^i,\bar{\gamma}^i_1)$ and $\overline{\Xi}_2(\bar{x}^i,\bar{\xi}^\alpha_1)$ vanish at the given point p for the particular choice of n-velocity or $(n-1)$-velocity. Note that the same coordinate system will not necessarily work at a given point p for every choice of velocity; that is, the fields A and Ξ need not be geodesic.

E. When an acceleration field determines a directing field

A curve structure need not determine a path structure; however, to every path structure, there corresponds a family of curve structures.[17]

Theorem 3.1: An acceleration field A determines a directing field Ξ iff A is of the form

$$A^i_2(x^i,\gamma^i_1)=B(x^i,\gamma^i_1)\gamma^i_1+C^i(x^i,\gamma^i_1)\,, \tag{3.11}$$

where $C^i(x^i,\gamma^i_1)$ does not contain a term proportional to γ^i_1 and

$$C^i(x^i,\lambda\gamma^i_1)=\lambda^2C^i(x^i,\gamma^i_1)\,. \tag{3.12}$$

Proof: For convenience, suppress the dependence of the fields on the coordinates x^i.

An acceleration field A determines a directing field Ξ iff for every $p\in M$, the $(n-1)$-acceleration ξ^α_2 determined by $A^i_2(\gamma^i_1)$ is the same as the $(n-1)$-acceleration determined by $A^i_2(\lambda\gamma^i_1)$;that is, ξ^α_2 depends only on ξ^α_1. The formula for ξ^α_2 in terms of γ^i_1 and γ^i_2 is

$$\xi^\alpha_2=(\gamma^n_1\gamma^\alpha_2-\gamma^\alpha_1\gamma^n_2)/(\gamma^n_1)^3\,. \tag{3.13}$$

Hence, the condition that A must satisfy may be stated as

$$\frac{\gamma^n_1A^\alpha_2(\gamma^i_1)-\gamma^\alpha_1A^n_2(\gamma^i_1)}{(\gamma^n_1)^3}=\frac{(\lambda\gamma^n_1)A^\alpha_2(\lambda\gamma^i_1)-(\lambda\gamma^\alpha_1)A^i_2(\lambda\gamma^i_1)}{(\lambda\gamma^n_1)^3}\,. \tag{3.14}$$

Since, in general, n charts are required to cover the direction fibers, the condition (3.14) may be more precisely stated as

$$\gamma_1^i [A^j_{\ 2}(\gamma_1^i) - (1/\lambda^2) A^j_{\ 2}(\lambda\gamma_1^i)]$$
$$= \gamma_1^j [A^i_{\ 2}(\gamma_1^i) - (1/\lambda^2) A^i_{\ 2}(\gamma_1^i)] , \tag{3.15}$$

for $i \neq j$. It follows from the transformation law (3.5) that

$$E^i(\gamma_1^i) = A^i_{\ 2}(\gamma_1^i) - (1/\lambda^2) A^i_{\ 2}(\lambda\gamma_1^i) \tag{3.16}$$

transforms according to

$$\bar{E}^i(\bar{\gamma}_1^i) = \bar{X}^i_{\ j} E^j(\gamma_1^i) . \tag{3.17}$$

The condition (3.15) states that the wedge product $\gamma_1 \wedge E(\gamma_1^i)$ vanishes which is equivalent to the condition that $E^i(\gamma_1^i)$ is proportional to γ_1^i (see Ref. 18).

An acceleration field A which satisfies (3.11) and (3.12) also satisfies (3.15) and hence determines a directing field Ξ given by

$$\Xi^\alpha_{\ 2}(\xi^\alpha_{\ 1}) = [\gamma_1^n C^\alpha(\gamma_1^i) - \gamma_1^\alpha C^n(\gamma_1^i)]/(\gamma_1^n)^3 , \tag{3.18}$$

because the terms proportional to γ_1^i drop out and (3.12) ensures that (3.18) depends only on $\xi^\alpha_{\ 1}$.

On the other hand, if an acceleration field A determines a directing field Ξ and hence satisfies (3.15), then any term of the form $B(x^i,\gamma_1^i)\gamma_1^i$ may be chosen arbitrarily and the term $C^i(x^i,\gamma_1^i)$ that does not contain a term proportional to γ_1^i must satisfy

$$\gamma_1^i [C^j(\gamma_1^i) - (1/\lambda^2) C^j(\lambda\gamma_1^i)]$$
$$= \gamma_1^j [C^i(\gamma_1^i) - (1/\lambda^2) C^i(\lambda\gamma_1^i)] , \tag{3.19}$$

for $i \neq j$. It follows that

$$C^i(\gamma_1^i) - (1/\lambda^2) C^i(\lambda\gamma_1^i) = 0 \tag{3.20}$$

since the left side must be linearly dependent on γ_1^i by (3.19) and yet by assumption cannot be a nonzero multiple of γ_1^i.

F. Acceleration fields which determine nongeodesic directing fields

It is important to emphasize that directing fields determined by acceleration fields A which satisfy the conditions (3.11) and (3.12) of Theorem 3.1 are *not*, in general, geodesic. Consider, however, the following well-known result.[19]

Theorem 3.2: If an acceleration field A satisfies the conditions (3.11) and (3.12) of Theorem 3.1, and if $C^i(x^i,\gamma_1^i)$ is C^2 in the variables γ_1^i, then the directing field determined by A is geodesic.

Proof: Differentiate (3.12) twice with respect to λ and set $\lambda = 0$ to obtain

$$C^i(x^i,\gamma_1^i) = \frac{1}{2} \frac{\partial^2 C^i(x^i,0)}{\partial\gamma_1^j \partial\gamma_1^k} \gamma_1^j \gamma_1^k , \tag{3.21}$$

from which geodesicity follows easily.

On the other hand, it readily follows from (3.12) that $C^i(x^i,\gamma_1^i)$ must be C^1 in the variables γ_1^i for all γ_1^i. It turns out that important, physically relevant acceleration fields are C^∞ in the variables γ_1^i for all γ_1^i except $\gamma_1^i = 0$. As a concrete example, consider the well-known one-parameter (Q/m) family of acceleration fields[20]

$$A^i_{\ 2}(\gamma_1^i) = B(\gamma_1^i)\gamma_1^i - \Gamma^i_{jk}\gamma_1^j\gamma_1^k + (Q/m)(g_{rs}\gamma_1^r\gamma_1^s)^{1/2} F^i_{\ j}\gamma_1^j , \tag{3.22}$$

where $B: L^1_{\ 1}(M) \to \mathbb{R}$, g is a Riemannian metric on M, Γ is the corrresponding affine structure, $F^i_{\ j}$ is the electromagnetic field tensor, Q is the electric charge, and m is the inertial mass. The directing field Ξ determined by the acceleration field (3.22) is given by

$$\Xi^\alpha_{\ 2}(\xi^\alpha_{\ 1}) = \xi^\alpha_{\ 1}[\Pi^n_{\rho\sigma}\xi^\rho_{\ 1}\xi^\sigma_{\ 1} + 2\Pi^n_{n\rho}\xi^\rho_{\ 1} + \Pi^n_{nn}] - [\Pi^\alpha_{\rho\sigma}\xi^\rho_{\ 1}\xi^\sigma_{\ 1} + 2\Pi^\alpha_{n\rho}\xi^\rho_{\ 1} + \Pi^\alpha_{nn}]$$
$$+ (Q/m)(g_{nn})^{1/2}[1 + 2\varphi_{n\beta}\xi^\beta_{\ 1} + \varphi_{\beta\gamma}\xi^\beta_{\ 1}\xi^\gamma_{\ 1}]^{1/2}[(F^\alpha_{\ n} + F^\alpha_{\ \rho}\xi^\rho_{\ 1}) - \xi^\alpha_{\ 1}(F^n_{\ n} + F^n_{\ \rho}\xi^\rho_{\ 1})] , \tag{3.23}$$

where the coefficients

$$\Pi^i_{jk} = \Gamma^i_{jk} - [1/(n+1)](\delta^i_j\Gamma_k + \delta^i_k\Gamma_j) \tag{3.24}$$

satisfy

$$\Pi^j_{jk} = 0 \tag{3.25}$$

and determines the projective structure of space-time, and where the coefficients

$$\varphi_{n\alpha} = g_{n\alpha}/g_{nn} , \quad \varphi_{\alpha\beta} = g_{\alpha\beta}/g_{nn} \tag{3.26}$$

determine the conformal structure of space-time. Since the factor $[1 + \varphi_{n\beta}\xi^\beta_{\ 1} + \varphi_{\beta\gamma}\xi^\beta_{\ 1}\xi^\gamma_{\ 1}]^{1/2}$ is not polynomial in the variables $\xi^\alpha_{\ 1}$, the directing field is clearly not geodesic. We have given more elaborate examples elsewhere.[21] It is easy to show that the acceleration field (3.22) is C^1 but not C^2 at $\gamma_1^i = 0$.

G. Compatibility with special relativity

The essential features of the special theory of relativity are incorporated into the general theory of relativity by the requirement that at each point $p \in M$, the microsymmetry group of the space-time metric is isomorphic to the Lorentz group, SO(1,$n-1$). As a consequence of this requirement, derivative geometric structures, such as the conformal, affine, and projective structures, have microsymmetry groups (at each point $p \in M$) the first-order part of which contains a subgroup isomorphic to the group SO(1,$n-1$). This observation motivates the following.

Definition: A space-time geometric structure field is compatible with the special theory of relativity (STR) iff its microsymmetry group at each point $p \in M$ has a first-order part which contains a subgroup that is isomorphic to the group SO(1,$n-1$).

The inertial structure of space-time is a geometric structure field. It may be either an acceleration or a directing field. In Sec. IV and V, it will be shown that such fields that are compatible with STR must be geodesic. In each case, the general result is proved by considering in turn the four possibilities for the first-order part of the microsymmetry group; namely, GL(n,$\mathbb{R}$), SL(n,$\mathbb{R}$), CO(1,$n-1$), and SO(1,$n-1$).

That only these four cases need to be considered follows from the fact that $GL(n,\mathbb{R})$ is the direct product of the dilation subgroup and $SL(n,\mathbb{R})$, and from the following two established results.

Theorem 3.3: The group $SO(p,q)$ is a maximal subgroup of $SL(n,\mathbb{R})$.

Remark: An analysis of the maximal subgroups of the classical groups has been given by Dynkin.[22] Fortunately the particular case of interest is listed in a table in the book by Gilmore.[23]

Theorem 3.4: If G is a subgroup of $SL(n,\mathbb{R})$ isomorphic to $SO(p,q)$, then G is conjugate to $SO(p,q)$.

Proof: The defining $(p+q)$-dimensional representation of $SO(p,q)$ is both real and self-contragredient. It is easy to show that all tensor representations and the irreducible components of these representations are also real and self-contragredient. The isomorphism $D:SO(p,q)\to G\subset SL(n,\mathbb{R})$ provides a real vector representation of $SO(p,q)$ which must be equivalent to an irreducible part of some tensor representation which is therefore self-contragredient. There exists a real symmetric bilinear invariant for the representation D which is unique up to a constant multiple.[24] The signature of this metric must be $p-q$ (or $q-p$), and the diagonalization procedure provides the coordinate transformation that maps each element of G into its conjugate in $SO(p,q)$.

IV. GEODESICITY OF STR COMPATIBLE ACCELERATION FIELDS

The group of jets $j_p^k f$ of diffeomorphisms $f: M\to M$ which satisfy $f(p)=p$ is denoted by G_p^k. A jet $j_p^2 f\in G_p^2$ with components (f_j^i, f_{jk}^i) is a microsymmetry of an acceleration field A at $p\in M$ iff[25]

$$A_2^i(f_j^i\gamma_1^j) = f_r^i A_2^r(\gamma_1^i) + f_{jk}^i\gamma_1^j\gamma_1^k . \tag{4.1}$$

For an infinitesimal microtransformation $(\delta_j^i+\epsilon F_j^i, \epsilon F_{jk}^i)$, the condition (4.1) becomes

$$F_j^k\gamma_1^j A_{2,k}^i(\gamma_1^i) = F_j^i A_2^j(\gamma_1^i) + F_{jk}^i\gamma_1^j\gamma_1^k . \tag{4.2}$$

The following theorem sets an upper limit to the degree of microisotropy that an acceleration field can possess.

Theorem 4.1: The microsymmetry group of an acceleration field is a subgroup of G_p^2 that is isomorphic to a *subgroup* of $G_n^1(GL(n,\mathbb{R}))$.

Proof: Write (4.1) as

$$f_{jk}^i\gamma_1^j\gamma_1^k = A_2^i(f_j^i\gamma_1^j) - f_r^i A_2^r(\gamma_1^i) . \tag{4.3}$$

Even if the field $A_2^i(\gamma_1^i)$ is not C^2 in the variables γ_1^i, the right side of (4.3) is C^2 since the left side is. Hence, the second-order components f_{jk}^i of a microsymmetry can be determined in terms of the field A and the first-order components f_j^i by differentiating (4.3) twice with respect to γ_1^i and setting $\gamma_1^i=0$.

The following well-known result shows that the maximal degree of microisotropy is attained by a geodesic acceleration field.

Theorem 4.2: The microsymmetry group of a geodesic acceleration field is a subgroup of G_p^2 that is isomorphic to G_n^1.

Proof: Substitute (3.6) into (4.1) to obtain the microsymmetry group element

$$(f_j^i, f_r^i\Gamma_{jk}^r - \Gamma_{rs}^i f_j^r f_k^s) . \tag{4.4}$$

Theorem 4.3: An acceleration field A which is at least C^1 in the variables γ_1^i and which has at every point $p\in M$ a microsymmetry group having a first-order part that contains the group of dilations is of the form

$$A_2^i(\gamma_1^i) = B_j^i\gamma_1^j - \Gamma_{jk}^i\gamma_1^j\gamma_1^k , \tag{4.5}$$

where B_j^i and Γ_{jk}^i depend only on p.

Proof: A microsymmetry which has a dilation for its first-order part has the form $(\lambda\delta_j^i, f_{jk}^i)$, where the f_{jk}^i are determined by λ and the field A. The condition (4.1) gives in this special case

$$\lambda A_2^i(\gamma_1^i) = A_2^i(\lambda\gamma_1^i) - f_{jk}^i\gamma_1^j\gamma_1^k . \tag{4.6}$$

Differentiating this equation with respect to λ and then setting $\lambda=0$, one obtains

$$A_2^i(\gamma_1^i) = A_{2,r}^i(0)\gamma_1^r - \frac{d}{d\lambda}f_{jk}^i(0)\gamma_1^j\gamma_1^k . \tag{4.7}$$

Theorem 4.4: If the first-order part of the microsymmetry group of an acceleration field A, which is at least C^1 in the variables γ_1^i, is isomorphic to either $GL(n,\mathbb{R})$ or $CO(1,n-1)$, then A is geodesic.

Proof: Both $GL(n,\mathbb{R})$ and $CO(1,n-1)$ contain the group of dilations. Hence the field A is given by (4.5). Together (4.1) and (4.5) yield

$$f_{jk}^i = f_r^i\Gamma_{jk}^r - \Gamma_{rs}^i f_j^r f_k^s \tag{4.8}$$

and

$$B_r^i f_j^r = f_r^i B_j^r . \tag{4.9}$$

From (4.9), it follows by Schur's lemma that

$$B_j^i = B\delta_j^i . \tag{4.10}$$

A term like $B\delta_j^i$ may always be removed from A by a suitable change of parameter.

Theorem 4.5: If the first-order part of the microsymmetry group of an acceleration field A which is at least C^1 in the variables γ_1^i is isomorphic to $SL(n,\mathbb{R})$, then A is geodesic.

Proof: By Theorem 4.1, the microsymmetries of an acceleration field A have the form $(f_j^i, S_{jk}^i(f_j^i))$. In Appendix A, it is shown that for the case of a microsymmetry group isomorphic to $SL(n,\mathbb{R})$, the second-order part F_{jk}^i of an infinitesimal microsymmetry is given by

$$F_{jk}^i = S_{jk\,r}^{i\,s} F_s^r , \tag{4.11}$$

where the $S_{jk\,r}^{i\,s}$ depend only on the point $p\in M$ and have the specific form given by (A16). Using a complete set of F_j^i, namely,

$$(F_j^i)_r^s = \delta_r^i\delta_j^s - (1/n)\delta_j^i\delta_r^s , \tag{4.12}$$

one obtains from (4.2)

$$\gamma_1^s A_{2,r}^i(\gamma_1^i) - (1/n)\delta_r^s\gamma_1^a A_{2,a}^i(\gamma_1^i) = \delta_r^i A_2^s(\gamma_1^i) - (1/n)\delta_r^s A_2^i(\gamma_1^i) + S_{jk\,r}^{i\,s}\gamma_1^j\gamma_1^k . \tag{4.13}$$

Define $B^i(\gamma_1^i)$ by

$$A_2^i(\gamma_1^i) = B^i(\gamma_1^i) - \hat{R}_{jk}^i\gamma_1^j\gamma_1^k . \tag{4.14}$$

Then (4.13) gives

$$\gamma_1^s B^i{}_{,r}(\gamma_1^j) - (1/n)\delta_r^s \gamma_1^a B^i{}_{,a}(\gamma_1^j) = \delta_r^i B^s(\gamma_1^j) - (1/n)\delta_r^s B^i(\gamma_1^j) + 2\frac{n^2+1}{n^2-1}\gamma_1^j \gamma_1^s R_r - \frac{2}{n}\frac{n^2+1}{n^2-1}\delta_r^s \gamma_1^j R_a \gamma_1^a . \tag{4.15}$$

Next, define $C^i(\gamma_1^j)$ by

$$B^i(\gamma_1^j) = C^i(\gamma_1^j) + 2[(n^2+1)/(n^2-1)]\gamma_1^j R_a \gamma_1^a . \tag{4.16}$$

Then (4.15) gives

$$\gamma_1^s C^i{}_{,r}(\gamma_1^j) - (1/n)\delta_r^s \gamma_1^a C^i{}_{,a}(\gamma_1^j) = \delta_r^i C^s(\gamma_1^j) - (1/n)\delta_r^s C^i(\gamma_1^j) . \tag{4.17}$$

From (4.13), it is clear that $A^i{}_2(\mathbf{0})$ and hence $B^i(\mathbf{0})$ and $C^i(\mathbf{0})$ vanish. In (4.17), choose $i = s \neq r$ without summing to obtain

$$\gamma_1^s C^s{}_{,r}(\gamma_1^j) = 0 \quad \text{(NO SUM)} . \tag{4.18}$$

Hence provided $\gamma_1^s \neq 0$,

$$C^s{}_{,r}(\gamma_1^j) = 0 . \tag{4.19}$$

However, $C^s{}_{,r}(\gamma_1^j)$ is at least C^0 since $A^i{}_2(\gamma_1^j)$ is at least C^1. Thus (4.19) holds for all γ_1^j; consequently, $C^s(\gamma_1^j)$ depends at most on the γ_1^s component of the n-velocity. For any fixed s, denote γ_1^s by u and $C^s(\gamma_1^j)$ by $f(u)$. Then choosing $i = s = r$ in (4.17) without summing, one obtains

$$u\frac{df}{du} = f . \tag{4.20}$$

Hence, $f(u) = ku$, and

$$C^s(\gamma_1^j) = k_s \gamma_1^s \quad \text{(no sum)} . \tag{4.21}$$

Then (4.17) gives

$$\gamma_1^s \delta_r^i k_i - (1/n)\delta_r^s k_i \gamma_1^i = \delta_r^i k_s \gamma_1^s - (1/n)\delta_r^s k_i \gamma_1^i \quad \text{(no sum)} . \tag{4.22}$$

Choosing $i = r \neq s$, one obtains

$$\gamma_1^s k_i = k_s \gamma_1^s \quad \text{(no sum)} . \tag{4.23}$$

Hence k_s is the same for all s and

$$C^i(\gamma_1^j) = C\gamma_1^j , \tag{4.24}$$

where C depends only on $p \in M$. Since such a term may always be removed from A by a suitable change of parameter, A is geodesic.

Theorem 4.6: If the first-order part of the microsymmetry group of an acceleration field A, which is at least C^1 in the variables γ_1^j, is isomorphic to SO(p,q) [hence, in particular, to SO(1,$n-1$)], then A is geodesic.

Proof: If an acceleration field A is a homogeneous quadratic in the variables γ_1^j with respect to some coordinate system, then it is a homogeneous quadratic in the variables γ_1^j with respect to any coordinate system, and is, moreover, geodesic. Since an active symmetry does not depend on the choice of coordinate system, the invariance condition (4.2) may be applied in that coordinate system in which the first-order part of the microsymmetry group is SO(p,q) in its standard form (see Theorem 3.4). Then, for an infinitesimal SO(p,q) transformation

$$F_{ab} = \eta_{al} F^l_b = -F_{ba} . \tag{4.25}$$

Also, the second-order part of the infinitesimal microsymmetry is given by

$$F^i_{jk} = (1/2!) S^{i\,ab}_{jk} F_{ab} , \tag{4.26}$$

where $S^{i\,ab}_{jk}$ has the specific form (B22) derived in Appendix B where the $\hat{R}^i_{jk}$, H^i, and V^i depend only on the point $p \in M$. The invariance condition (4.2) together with (4.25) and (4.26) yields

$$(\gamma_1^a \eta^{bk} - \gamma_1^b \eta^{ak}) A^i_{2,k}(\gamma_1^j) + (\eta^{ia} A^b_2(\gamma_1^j) - \eta^{ib} A^a_2(\gamma_1^j)) + S^{i\,ab}_{jk} \gamma_1^j \gamma_1^k = 0 . \tag{4.27}$$

Define the field B^i by

$$A^i_2(\gamma_1^j) = B^i(\gamma_1^j) - \hat{R}^i_{jk} \gamma_1^j \gamma_1^k + (2/n)\eta^{im}\eta_{kl}\gamma_1^k \hat{R}^l_{mj}\gamma_1^j - \frac{(n+1)(n-2)}{n(n-1)(n+2)}[\eta_{jk}\gamma_1^j\gamma_1^k H^i + 2\gamma_1^j \gamma_1^p H_p] + 2\frac{(n+1)(n-2)}{(n-1)(n+2)}\left[\frac{1}{n}\eta_{jk}\gamma_1^j\gamma_1^k V^i - \gamma_1^i \gamma_1^p V_p\right] . \tag{4.28}$$

It follows from (B22), (4.27), and (4.28) that $B^i(\gamma_1^j)$ satisfies

$$(\gamma_1^a \eta^{bk} - \gamma_1^b \eta^{ak}) B^i{}_{,k}(\gamma_1^j) + (\eta^{ia} B^b(\gamma_1^j) - \eta^{ib} B^a(\gamma_1^j)) = 0 . \tag{4.29}$$

This condition is just the infinitesimal version of the invariance condition

$$B^i(\Lambda^i{}_j \gamma_1^j) = \Lambda^i_j B^j(\gamma_1^j) , \tag{4.30}$$

where $\Lambda \in$ SO(p,q).

For the following discussion, the summation convention is suspended. In (4.29), choose $i = a \neq b$ and relabel $i \to r$ and $a \to i$ to obtain

$$B^i = \gamma_1^i B^r{}_{,r} - \eta^{ii}\eta^{rr}\gamma_1^r B^r{}_{,i} \quad (r \neq i) . \tag{4.31}$$

Next, take a, b, and i all different in (4.29) and use the relabeling $a \to i$ and $i \to r$ to obtain

$$\gamma_1^i \eta^{ss} B^r{}_{,s} = \gamma_1^s \eta^{ii} B^r{}_{,i} , \quad i \neq r , \quad i \neq s , \quad r \neq s . \tag{4.32}$$

Then

$$B^r{}_{,i} = \eta^{ii}\gamma_1^i \eta^{ss} B^r{}_{,s}/\gamma_1^s , \quad i \neq r , \quad i \neq s , \quad r \neq s . \tag{4.33}$$

Hence, (4.31) and (4.33) yield

$$B^i(\gamma_1^j) = \gamma_1^i H(\gamma_1^j) . \tag{4.34}$$

The summation convention is reinstated. Since $B^i(\gamma_1^j)$ is at least C^1 in the variables γ_1^j, $H(\gamma_1^j)$ is at least C^1 in the variables γ_1^j for $\boldsymbol{\gamma}_1 \neq \mathbf{0}$. The example,

$$H(\gamma_1^j) = (\eta_{jk}\gamma_1^j \gamma_1^k)^m \quad (0 < m \leqslant \tfrac{1}{2}) , \tag{4.35}$$

shows that $H(\gamma_1^j)$ need not be C^1 at $\boldsymbol{\gamma}_1 = \mathbf{0}$; however, that $H(\gamma_1^j)$ is C^0 may be shown as follows. Let u^i be any fixed nonzero vector. It is clear from (4.31) that $B^i(\mathbf{0}) = 0$. The difference quotient for $B^i(\boldsymbol{\gamma}_i)$ at $\boldsymbol{\gamma}_1 = \mathbf{0}$ in the direction $\mathbf{u}$ is

$$B^i(\lambda \mathbf{u})/\lambda = \lambda u^i H(\lambda \mathbf{u})/\lambda = u^i H(\lambda \mathbf{u}) . \tag{4.36}$$

Since $B^i(\gamma_1^j)$ is C^1,

$$u^i \lim_{\lambda \to 0} H(\lambda \mathbf{u}) = u^k B^i{}_{,k}(\mathbf{0}) . \tag{4.37}$$

Clearly, $B^i{}_{,k}(\mathbf{0}) = \delta^i_k B$, where B depends on $p \in M$ but is independent of $\mathbf{u}$. Hence

$$\lim_{\lambda\to 0} H(\lambda \mathbf{u}) = B\,. \tag{4.38}$$

The field A is geodesic because a term such as (4.34) can always be eliminated by means of a suitable change of parameter and the other terms on the right side of (4.28) constitute a homogeneous quadratic in the variables γ_1^i.

V. GEODESICITY OF STR COMPATIBLE DIRECTING FIELDS

A jet $j_p^2 f \in G_p^2$ is a microsymmetry of a directing field Ξ at $p \in M$ iff[25]

$$\Xi_2^\alpha\left(\frac{f_i^\alpha \xi_1^i}{f_i^n \xi_1^i}\right) = \frac{f_\beta^\alpha \Xi_2^\beta(\xi_1^\alpha) f_i^n \xi_1^i - f_\beta^n \Xi_2^\beta(\xi_1^\alpha) f_i^\alpha \xi_1^i}{(f_i^n \xi_1^i)^3} + \frac{f_{jk}^\alpha \xi_1^j \xi_1^k f_i^n \xi_1^i - f_{jk}^n \xi_1^j \xi_1^k f_i^\alpha \xi_1^i}{(f_i^n \xi_1^i)^3}\,, \tag{5.1}$$

where the convention $\xi_1^n = 1$ has been used in order to express the result in a compact form. For an infinitesimal microtransformation, the condition (5.1) becomes

$$\Xi_{2,\beta}^\alpha(\xi_1^\alpha)[F_\gamma^\beta \xi_1^\gamma + F_n^\beta - \xi_1^\beta(F_\gamma^n \xi_1^\gamma + F_n^n)] + 2\Xi_2^\alpha(\xi_1^\alpha)[F_\gamma^n \xi_1^\gamma + F_n^n] + \Xi_2^\beta(\xi_1^\alpha)[F_{\beta\gamma}^n \xi_1^\alpha - F_\beta^\alpha]$$
$$= F_{\rho\sigma}^\alpha \xi_1^\rho \xi_1^\sigma + 2F_{n\rho}^\alpha \xi_1^\rho + F_{nn}^\alpha - \xi_1^\alpha[F_{\rho\sigma}^n \xi_1^\rho \xi_1^\sigma + 2F_{n\rho}^n \xi_1^\rho + F_{nn}^n]\,. \tag{5.2}$$

Theorem 5.1: Microtransformations of the form $(\delta_j^i, \delta_j^i a_k + \delta_k^i a_j)$ are microsymmetries for any directing field.

Remark: The result follows easily from (5.1). Moreover,

$$(f_j^i, 0)(\delta_j^i, \hat{f}_{jk}^i) = (f_j^i, f_r^i \hat{f}_{jk}^r) \tag{5.3}$$

and since

$$(\delta_j^i, \hat{f}_{jk}^i)(\delta_j^i, \delta_j^i f_k + \delta_k^i f_j) = (\delta_j^i, \hat{f}_{jk}^i + \delta_j^i f_k + \delta_k^i f_j)\,, \tag{5.4}$$

attention may be restricted to microsymmetries $(f_j^i, f_r^i \hat{f}_{jk}^r)$ which satisfy $\hat{f}_{jk}^k = 0$.

The subgroup of G_n^2 consisting of the elements of the form

$$(a_j^i, a_j^i a_k + a_k^i a_j)$$

is denoted by P_n^2. This group is characteristic for geodesic directing fields.

Theorem 5.3: A directing field is geodesic iff at every $p \in M$ its microsymmetry group is a subgroup of G_p^2 isomorphic to P_n^2.

Remark: This theorem is a combination of Theorem 5 and Theorem 6 of Ref. 4. The directing field Π is then given by (3.9) and its microsymmetries have the form

$$(f_j^i, f_r^i \Pi_{jk}^r - \Pi_{rs}^i f_j^r f_k^s + f_j^i f_k + f_k^i f_j)\,. \tag{5.5}$$

Note that for this case

$$\hat{f}_{jk}^i = \Pi_{jk}^i - f^{-1}{}_l^i \Pi_{rs}^l f_j^r f_k^s\,, \tag{5.6}$$

which does satisfy $\hat{f}_{jk}^k = 0$.

The degree of microisotropy exhibited by geodesic directing fields is maximal for directing fields.

Theorem 5.4: The microsymmetry group of a directing field Ξ is a subgroup of G_p^2 that is isomorphic to a subgroup of P_n^2.

Proof: In Appendix C, it is shown that the traceless part $\hat{F}_{jk}^i$ of the second-order part F_{jk}^i of an infinitesimal microsymmetry of a directing field is determined by the first-order part F_j^i of the infinitesimal microsymmetry and by derivatives of $\Xi_2^\alpha(x^i, \xi_1^\alpha)$ with respect to ξ_1^α evaluated at $\xi_1^\alpha = 0$.

Theorem 5.5: If at every point $p \in M$ the first-order part of the microsymmetry group of a directing field Ξ is isomorphic to $GL(n,\mathbb{R})$ or to $CO(1,n-1)$, then Ξ is geodesic.

Remark: This result follows from the fact that the group of dilations is a subgroup of both $GL(n,\mathbb{R})$ and $CO(1,n-1)$; so that Theorem 6 of Ref. 4 applies. This theorem states that a directing field which admits at every $p \in M$ a microsymmetry $j_p^2 f \in G_p^2$ with $f_j^i = \lambda \delta_j^i$ and $\lambda \neq 1$ is geodesic.

Theorem 5.6: If at every $p \in M$ the first-order part of the microsymmetry group of a directing field Ξ is isomorphic to $SL(n,\mathbb{R})$, then Ξ is geodesic.

Proof: Decomposing (4.12) into the various possible index combinations, one obtains

$$(F_\gamma^\beta)_\rho^\sigma = \delta_\rho^\beta \delta_\gamma^\sigma - (1/n)\delta_\gamma^\beta \delta_\rho^\sigma\,, \quad (F_\gamma^\beta)_n^n = -(1/n)\delta_\gamma^\beta\,,$$
$$(F_n^\beta)_\rho^n = \delta_\rho^\beta\,, \quad (F_\gamma^n)_n^\sigma = \delta_\gamma^\sigma\,, \tag{5.7}$$
$$(F_n^n)_\rho^\sigma = -(1/n)\delta_\rho^\sigma\,, \quad (F_n^n)_n^n = -(n-1)/n\,.$$

The traceless second-order part of F_{jk}^i is given by

$$(\hat{F}_{jk}^i)_r^s = \hat{S}_{jkr}^{is}\,, \tag{5.8}$$

where $\hat{S}_{jkr}^{is}$ is given by (A17). Then (5.2) splits up into four conditions corresponding to the choices (ρ,σ), (ρ,n), (n,σ), and (n,n) for the indices (r,s). The simplest choice $(r,s) = (\rho,n)$ gives

$$\Xi_{2,\rho}^\alpha(\xi_1^\alpha) = \delta_\rho^\alpha(\hat{R}_{\mu\nu}^n \xi_1^\mu \xi_1^\nu + 2\hat{R}_{n\nu}^n \xi_1^\nu + \hat{R}_{nn}^n) - 2\hat{R}_{\nu\rho}^\alpha \xi_1^\nu - 2\hat{R}_{n\rho}^\alpha + \xi_1^\alpha(2\hat{R}_{\nu\rho}^n \xi_1^\nu + 2R_{n\rho}^n)\,. \tag{5.9}$$

Define $B^\alpha(\xi_1^\alpha)$ by

$$\Xi_2^\alpha(\xi_1^\alpha) = B^\alpha(\xi_1^\alpha) + \xi_1^\alpha(\hat{R}_{\mu\nu}^n \xi_1^\mu \xi_1^\nu + 2\hat{R}_{n\nu}^n \xi_1^\nu + \hat{R}_{nn}^n) - (\hat{R}_{\mu\nu}^\alpha \xi_1^\mu \xi_1^\nu + 2\hat{R}_{n\nu}^\alpha \xi_1^\nu + \hat{R}_{nn}^\alpha)\,. \tag{5.10}$$

Then (5.9) and (5.10) together give

$$B_{,\rho}^\alpha(\xi_1^\alpha) = 0\,. \tag{5.11}$$

If the above procedure is repeated for the choice $(r,s) = (\rho,\sigma)$, one obtains

$$\xi_1^\sigma B_{,\rho}^\alpha(\xi_1^\alpha) - \delta_\rho^\alpha B^\sigma(\xi_1^\alpha) - (1/n)\delta_\rho^\sigma B^\alpha(\xi_1^\alpha) = 0\,. \tag{5.12}$$

Hence

$$B^\alpha(\xi_1^\alpha) = 0\,. \tag{5.13}$$

Consequently, the field Ξ is geodesic.

Theorem 5.7: If for every $p \in M$ the first-order part of the microsymmetry group of a directing field Ξ is isomorphic to

SO(p,q) [hence, in particular, to SO(1,$n-1$)], then Ξ is geodesic.

Proof: To show that Ξ is geodesic, it is sufficient to show that at any point $p\in M$ and for any $(n-1)$-velocity ξ_1^α, the function $\Xi_2^\alpha(x^i(p),\xi_1^\alpha)$ is a cubic in the variables ξ_1^α of the form (3.9) because if Ξ has that form in one coordinate system, it will have that form in all coordinate systems.[26] Since an active microsymmetry is independent of the choice of coordinate system, the infinitesimal microinvariance condition (5.2) may be employed in the coordinate system in which the first-order part of the microsymmetry group is SO(p,q) in its standard form. An infinitesimal microtransformation is $(\delta_j^i+\epsilon F_j{}^i,\epsilon F_{jk}^{\ \ i})$, where (4.25) and (4.26) hold. A complete set of such transformations is given by

$$(F_{jk})^{rs}=\delta_j^r\delta_k^s-\delta_k^r\delta_j^s\,. \tag{5.14}$$

Then (5.2), (5.14), (4.25), and (4.26) yield the constraints for $(r,s)=(\mu,\nu)$,

$$\begin{aligned}&\Xi^\alpha_{2,\beta}(\xi_1^\alpha)[\eta^{\beta\mu}\xi_1^{\ \nu}-\eta^{\beta\nu}\xi_1^{\ \mu}]-(\eta^{\alpha\mu}\Xi^\nu_{\ 2}(\xi_1^\alpha)-\eta^{\alpha\nu}\Xi^\mu_{\ 2}(\xi_1^\alpha))\\&\quad=S_{\rho\sigma}^{\ \ \alpha\ \ \mu\nu}\xi_1^{\ \rho}\xi_1^{\ \sigma}+2S_{n\rho}^{\ \ \alpha\ \ \mu\nu}\xi_1^{\ \rho}+S_{nn}^{\ \ \alpha\ \ \mu\nu}\\&\qquad-\xi_1^\alpha[S_{\rho\sigma}^{\ \ n\ \ \mu\nu}\xi_1^{\ \rho\sigma}+2S_{n\rho}^{\ \ n\ \ \mu\nu}\xi_1^{\ \rho}+S_{nn}^{\ \ n\ \ \mu\nu}]\,,\end{aligned} \tag{5.15}$$

and for $(r,s)=(\mu,n)$,

$$\begin{aligned}&\Xi^\alpha_{2,\beta}(\xi_1^\alpha)[\eta^{\beta\mu}+\xi_1^{\ \beta}\xi_1^{\ \mu}\eta^{nn}]-2\eta^{nn}\xi_1^{\ \mu}\Xi^\alpha_{\ 2}(\xi_1^\alpha)\\&\qquad-\eta^{nn}\xi_1^{\ \alpha}\Xi^\mu_{\ 2}(\xi_1^\alpha)\\&\quad=S_{\rho\sigma}^{\ \ \alpha\ \ \mu n}\xi_1^{\ \rho}\xi_1^{\ \sigma}+2S_{n\rho}^{\ \ \alpha\ \ \mu n}\xi_1^{\ \rho}+S_{nn}^{\ \ \alpha\ \ \mu n}\\&\qquad-\xi_1^\alpha[S_{\rho\sigma}^{\ \ n\ \ \mu n}\xi_1^{\ \rho}\xi_1^{\ \sigma}+2S_{n\rho}^{\ \ n\ \ \mu n}\xi_1^{\ \rho}+S_{nn}^{\ \ n\ \ \mu n}]\,.\end{aligned} \tag{5.16}$$

With reference to (4.28), define

$$\begin{aligned}\Gamma_{jk}^i&=\hat R_{jk}^{\ \ i}-(1/n)\eta^{im}[\eta_{jl}\hat R_{mk}^{\ \ l}+\eta_{kl}\hat R_{mj}^{\ \ l}]\\&\quad+\frac{(n+1)(n-2)}{n(n-1)(n+2)}[\eta_{jk}H^i+\delta_j^iH_k+\delta_k^iH_j]\\&\quad+\frac{(n+1)(n-2)}{(n-1)(n+2)}[(2/n)\eta_{jk}V^i-\delta_j^iV_k-\delta_k^iV_j]\,,\end{aligned} \tag{5.17}$$

and define Π_{jk}^i by

$$\Gamma_{jk}^i=\Pi_{jk}^i+[1/(n+1)](\delta_j^i\Gamma_k+\delta_k^i\Gamma_j)\,, \tag{5.18}$$

where $\Pi_{rk}^{\ \ r}=0$. Then define the field $B^\alpha(\xi_1^\alpha)$ by

$$\Xi_2^\alpha(\xi_1^\alpha)=B^\alpha(\xi_1^\alpha)+\Pi_2^\alpha(\xi_1^\alpha)\,, \tag{5.19}$$

where $\Pi_2^\alpha(\xi_1^\alpha)$ is given by (3.9). Then (5.15), (5.16), and (5.19) yield

$$\begin{aligned}&\xi_1^{\ \mu}\eta^{\nu\beta}B^\alpha_{\ ,\beta}(\xi_1^\alpha)-\xi_1^{\ \nu}\eta^{\mu\beta}B^\alpha_{\ ,\beta}(\xi_1^\alpha)+\eta^{\alpha\mu}B^\nu(\xi_1^\alpha)\\&\quad-\eta^{\alpha\nu}B^\mu(\xi_1^\alpha)=0\end{aligned} \tag{5.20}$$

and

$$(\eta^{\mu\beta}+\eta^{nn}\xi_1^{\ \mu}\xi_1^{\ \beta})B^\alpha_{\ ,\beta}(\xi_1^\alpha)=\eta^{nn}(2\xi_1^{\ \mu}B^\alpha(\xi_1^\alpha)-\xi_1^\alpha B^\mu(\xi_1^\alpha))\,. \tag{5.21}$$

It is obvious that the terms involving $S_{jk}^{\ \ i\ \ ab}$ will drop out after the substitution (5.19) because they drop out in the acceleration field case and because (5.1) is a direct consequence of (4.1) and (3.18).

By means of the same argument used to derive (4.34) and (4.38), it follows from (5.21) that

$$B^\alpha(\xi_1^\alpha)=\xi_1^\alpha H(\xi_1^\alpha)\,, \tag{5.22}$$

where $H(\xi_1^\alpha)$ is C^0 in the variables ξ_1^α. From (5.21), it follows that

$$\begin{aligned}\eta^{\mu\beta}B^\alpha_{\ ,\beta}(\xi_1^\alpha)&=\eta^{nn}(2\xi_1^{\ \mu}B^\alpha(\xi_1^\alpha)-\xi_1^\alpha B^\mu(\xi_1^\alpha)\\&\quad+\xi_1^{\ \mu}\xi_1^{\ \beta}B^\alpha_{\ ,\beta}(\xi_1^\alpha))\,.\end{aligned} \tag{5.23}$$

Hence,

$$\begin{aligned}&\xi_1^{\ \mu}\eta^{\nu\beta}B^\alpha_{\ ,\beta}(\xi^\alpha)-\xi_1^{\ \nu}\eta^{\mu\beta}B^\alpha_{\ ,\beta}(\xi_1^\alpha)\\&\quad=-\eta^{nn}\xi_1^\alpha(\xi_1^{\ \mu}B^\nu(\xi_1^\alpha)-\xi_1^{\ \nu}B^\mu(\xi_1^\alpha))\,.\end{aligned} \tag{5.24}$$

Together (5.20) and (5.24) give

$$\begin{aligned}&\eta^{nn}\xi_1^\alpha(\xi_1^{\ \mu}B^\nu(\xi_1^\alpha)-\xi_1^{\ \nu}B^\mu(\xi_1^\alpha))\\&\quad=\eta^{\alpha\mu}B^\nu(\xi_1^\alpha)-\eta^{\alpha\nu}B^\mu(\xi_1^\alpha)\,.\end{aligned} \tag{5.25}$$

Then (5.22) and (5.25) yield

$$\eta^{\alpha\mu}\xi_1^{\ \nu}H(\xi_1^\alpha)=\eta^{\alpha\nu}\xi_1^{\ \mu}H(\xi_1^\alpha)\,. \tag{5.26}$$

Consequently, $H(\xi_1^\alpha)=0$ and Ξ is geodesic.

VI. UNIQUENESS OF THE PROJECTIVE STRUCTURE

In Secs. IV and V, it was proved that any equation of motion structure that has a sufficient degree of microisotropy to be compatible with STR must be geodesic and hence must define a projective structure on space-time. In this section, it is proved that such a structure must be unique for otherwise a subspace structure exists in some region of space-time.

The causal structure of space-time is determined by a conformal structure which may be described locally by an equivalence class of metric tensors

$$\{e^{\phi(x)}g_{ij}(x)|\phi:\mathbb{R}^4\to\mathbb{R}\}\,. \tag{6.1}$$

This first-order structure determines a unique sequence of prolongations to arbitrarily high order. The second-order structure is characterized by the conformal coefficients[11]

$$\begin{aligned}K_{jk}^{\ \ i}&=\tfrac12 g^{ir}(g_{rj,k}+g_{rk,j}-g_{jk,r})\\&\quad-(1/2n)(\delta_j^ig^{rs}g_{rs,k}+\delta_k^ig^{rs}g_{rs,j}-g_{jk}g^{it}g^{rs}g_{rs,t})\,.\end{aligned} \tag{6.2}$$

which satisfy $K_{kj}^{\ \ k}=0$ and are independent of the choice of gauge $\phi:\mathbb{R}^4\to\mathbb{R}$.

The set of projective structures that are physically compatible with a given conformal structure is severely limited by the following theorem.

Theorem 6.1: In order that it be impossible for a material body governed by a projective structure Π to break the light barrier determined by a given conformal structure (6.1), it is necessary and sufficient that the projective coefficients Π_{jk}^i be given by

$$\Pi_{jk}^i=K_{jk}^{\ \ i}+\frac1n\left[\frac{1}{n+1}(\delta_j^i\Gamma_k+\delta_k^i\Gamma_j)-g_{jk}g^{ir}\Gamma_r\right], \tag{6.3}$$

where Γ_k transforms as does the trace of an affine connection. Moreover, the projective and conformal structures then define a Weyl structure with an affine structure given by

$$\Gamma^i_{jk} = \Pi^i_{jk} + [1/(n+1)](\delta^i_j\Gamma_k + \delta^i_k\Gamma_j)$$
$$= K^i_{jk} + (1/n)(\delta^i_j\Gamma_k + \delta^i_k\Gamma_j - g_{jk}g^{ir}\Gamma_r]\,. \tag{6.4}$$

Remark: This theorem was first proved by Ehlers, Pirani, and Schild.[2] A complementary geometric derivation of the compatibility condition has been presented in one of our previous papers.[27] Note that (6.3) follows easily from (6.4).

The following theorem shows that in the context of GTR it is not possible for two distinct projective structures to coexist on space-time.

Theorem 6.2: Let Π and $\tilde{\Pi}$ be two projective structures that are distinct throughout some region of space-time. Suppose that both of these projective structures are compatible with the conformal causal structure of space-time in the sense that they both satisfy a relation of the form (6.3). Then, throughout the given region, there exists a subspace structure.[28]

Proof: From (6.3), it is evident that the only way that Π and $\tilde{\Pi}$ can be distinct is to have

$$\Gamma_k \neq \tilde{\Gamma}_k\,, \tag{6.5}$$

since K^i_{jk} and $g_{jk}g^{ir}$ are common to both Π and $\tilde{\Pi}$. The subspace structure is defined by the covector field

$$\omega_k = \Gamma_k - \tilde{\Gamma}_k\,, \tag{6.6}$$

which is nonvanishing throughout the given region. Note that if Π and $\tilde{\Pi}$ are continuous and differ at an event p, they must differ throughout some open neighborhood of the event p.

ACKNOWLEDGMENT

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.

APPENDIX A: SUBGROUPS OF G^2_n ISOMORPHIC TO SL(n,$\mathbb{R}$)

The Lie group G^2_n is the set of all jets $j^2_0 f$ where $f:\mathbb{R}^n\to\mathbb{R}^n$ is a diffeomorphism which satisfies $f(\mathbf{0}) = \mathbf{0}$ (see Ref 29). The Lie algebra $\mathcal{G}^2_n$ is spanned by $(E^{\,j}_i, E^{\,lm}_k)$ which satisfy the commutation relations

$$[E^{\,j}_i, E^{\,l}_k] = \delta^j_k E^{\,l}_i - \delta^l_i E^{\,j}_k\,,$$
$$[E^{\,j}_i, E^{\,lm}_k] = \delta^j_k E^{\,lm}_i - \delta^l_i E^{\,jm}_k - \delta^m_i E^{\,jl}_k\,, \tag{A1}$$
$$[E^{\,jk}_i, E^{\,mn}_l] = 0\,.$$

For an acceleration field, the second-order part of a microsymmetry is a function of the first-order part (Theorem 4.1). Thus the microsymmetry group is isomorphic to a subgroup of G^2_n which consists of elements of the form $(f^{\,i}_j, S^{\,i}_{jk}(f^{\,i}_j))$. From the group product for G^2_n, it follows that

$$S^{\,i}_{jk}(f^{\,i}_r h^{\,r}_j) = f^{\,i}_r S^{\,r}_{jk}(h^{\,i}_j) + S^{\,i}_{rs}(f^{\,i}_j) h^{\,r}_j h^{\,s}_k\,. \tag{A2}$$

For the case in which the subgroup is isomorphic to the group G^1_n, the function $S^{\,i}_{jk}(f^{\,i}_j)$ is given by the second part of (4.4).

From (A2), $S^{\,i}_{jk}(\delta^i_j) = 0$; consequently, for infinitesimal group elements

$$S^{\,i}_{jk}(\delta^i_j + \epsilon F^{\,i}_j) = \epsilon S^{\,i\ \ s}_{jk\ r} F^{\,r}_s\,. \tag{A3}$$

The Lie algebra sl(n,$\mathbb{R}$) of SL(n,$\mathbb{R}$)$\subset G^1_n$ is spanned by

$$\hat{E}^{\,j}_i = E^{\,j}_i - (1/n)E^{\,a}_a\delta^j_i\,, \tag{A4}$$

which also satisfy

$$[\hat{E}^{\,j}_i, \hat{E}^{\,l}_k] = \delta^j_k\hat{E}^{\,l}_i - \delta^l_i\hat{E}^{\,j}_k\,. \tag{A5}$$

Moreover,

$$[\hat{E}^{\,j}_i, E^{\,lm}_k] = \delta^j_k E^{\,lm}_i - \delta^l_i E^{\,jm}_k - \delta^m_i E^{\,lj}_k + (1/n)\delta^j_i E^{\,lm}_k\,. \tag{A6}$$

The generators of a subgroup of G^2_n which is isomorphic to SL(n,$\mathbb{R}$) have the form

$$\hat{H}^{\,j}_i = \hat{E}^{\,j}_i + \tfrac{1}{2} S^{\,r\ \ j}_{st\ \ i} E^{\,st}_r\,, \tag{A7}$$

where

$$S^{\,r\ \ a}_{st\ \ a} = 0\,. \tag{A8}$$

The requirement that the generators $\hat{H}^{\,j}_i$ satisfy the same commutation relations (A5) as the generators $\hat{E}^{\,j}_i$ yields the constraint

$$\delta^r_i S^{\,j\ \ l}_{st\ \ k} - \delta^j_s S^{\,r\ \ l}_{it\ \ k} - \delta^j_t S^{\,r\ \ l}_{si\ \ k} + (1/n)\delta^j_i S^{\,r\ \ l}_{st\ \ k}$$
$$- \delta^r_k S^{\,l\ \ j}_{st\ \ i} + \delta^l_s S^{\,r\ \ j}_{kt\ \ i} + \delta^l_t S^{\,r\ \ j}_{sk\ \ i} - (1/n)\delta^l_k S^{\,r\ \ j}_{st\ \ i}$$
$$= \delta^j_k S^{\,r\ \ l}_{st\ \ i} - \delta^l_i S^{\,r\ \ j}_{st\ \ k}\,. \tag{A9}$$

Contraction with respect to the indices i and r gives

$$(n + 1/n)S^{\,r\ \ l}_{st\ \ k} = \delta^r_s S^{\,a\ \ l}_{at\ \ k} + \delta^r_t S^{\,a\ \ l}_{as\ \ k} + \delta^r_k S^{\,a\ \ l}_{st\ \ a}$$
$$- \delta^l_s S^{\,a\ \ r}_{kt\ \ a} - \delta^l_t S^{\,a\ \ r}_{sk\ \ a} + (1/n)\delta^l_k S^{\,a\ \ r}_{st\ \ a}\,. \tag{A10}$$

The relation (A8) can also be obtained from (A10) by contraction on k and l followed by contraction on r and s.

Contraction of (A10) with respect to r and s gives

$$S^{\,a\ \ l}_{at\ \ k} = [n/(n-1)]\delta^l_t S^{\,a\ \ b}_{bk\ \ a} - [1/(n-1)]\delta^l_k S^{\,a\ \ b}_{bt\ \ a}\,. \tag{A11}$$

Contraction of (A11) with respect to t and l gives

$$S^{\,a\ \ b}_{ab\ \ k} = (n+1)S^{\,a\ \ b}_{bk\ \ a}\,. \tag{A12}$$

Define

$$R^{\,i}_{jk} = [n/(n^2+1)]S^{\,a\ \ i}_{jk\ \ a}\,. \tag{A13}$$

Then, (A10) and (A11) give, after a relabeling of indices,

$$S^{\,i\ \ s}_{jk\ \ r} = \delta^i_r R^{\,s}_{jk} - \delta^s_j R^{\,i}_{kr} - \delta^s_k R^{\,i}_{jr} + (1/n)\delta^s_r R^{\,i}_{jk}$$
$$+ \frac{n}{n-1}(\delta^i_j\delta^s_k + \delta^i_k\delta^s_j) R^{\,a}_{ar}$$
$$- \frac{1}{n-1}\delta^s_r(\delta^i_j R^{\,a}_{ak} + \delta^i_k R^{\,a}_{aj})\,. \tag{A14}$$

Finally, set

$$R_k = R^{\,a}_{ak}\,, \quad R^{\,i}_{jk} = \hat{R}^{\,i}_{jk} + [1/(n+1)](\delta^i_j R_k + \delta^i_k R_j)\,, \tag{A15}$$

where $\hat{R}^{\,i}_{jk}$ is traceless. Then

$$S^{\,i\ \ s}_{jk\ \ r} = \delta^{\,i}_r \hat{R}^{\,s}_{jk} - \delta^s_j\hat{R}^{\,i}_{kr} - \delta^s_k \hat{R}^{\,i}_{jr} + (1/n)\delta^s_r \hat{R}^{\,i}_{jk}$$
$$+ \frac{n^2+1}{n^2-1}(\delta^i_j\delta^s_k + \delta^i_k\delta^s_j) R_r$$
$$- \frac{1}{n}\frac{n^2+1}{n^2-1}\delta^s_r(\delta^i_j R_k + \delta^i_k R_j)\,. \tag{A16}$$

Let $\hat{S}^{\,i\ \ s}_{jk\ \ r}$ be the part of $S^{\,i\ \ s}_{jk\ \ r}$ that is traceless with respect to contraction on i and j. Then

$$\hat{S}^{\,i\ \ s}_{jk\ \ r} = \delta^i_r \hat{R}^{\,s}_{jk} - \delta^s_j \hat{R}^{\,i}_{kr} - \delta^s_k \hat{R}^{\,i}_{jr} + (1/n)\delta^s_r \hat{R}^{\,i}_{jk}\,. \tag{A17}$$

The above derivation shows that any solution of (A9) must have the form (A16). That (A16) is the general solution of (A9) may be proved by direct substitution.

APPENDIX B: SUBGROUPS OF G_n^2 ISOMORPHIC TO SO(p,q)

Because of Theorem 3.4, it may be assumed without loss of generality that the first-order part of the subgroup of G_n^2 is SO(p,q) in its standard form. Then, the generators of its Lie algebra are

$$L^{ij} = \eta^{ir}E_r^{\ j} - \eta^{jr}E_r^{\ i}, \tag{B1}$$

where η_{ij} and η^{ij} are diagonal and the diagonal entries η_{ii} and η^{ii} are $+1$ for $1 \leqslant i \leqslant p$ and -1 for $p+1 \leqslant i \leqslant p+q$. The Lie algebra of G_n^2 is spanned by $(E_i^{\ j}, E_k^{\ lm})$ which satisfy the commutation relations (A1). The L^{ij} satisfy the commutation relations

$$[L^{ij}, L^{kl}] = -\eta^{ik}L^{\ jl} - \eta^{jl}L^{\ ik} + \eta^{il}L^{\ jk} + \eta^{jk}L^{\ il} \tag{B2}$$

and

$$[L^{ij}, E_k^{\ lm}] = (L^{ij})_k^{\ r}E_r^{\ lm} - (L^{ij})_r^{\ l}E_k^{\ rm} - (L^{ij})_r^{\ m}E_k^{\ lr}, \tag{B3}$$

where

$$(L^{ij})_s^{\ r} = \eta^{ir}\delta_s^{\ j} - \eta^{jr}\delta_s^{\ i}. \tag{B4}$$

It follows from the argument presented at the beginning of Appendix A that the generators of a subgroup of G_n^2 which is isomorphic to SO(p,q) have the form

$$H^{rs} = L^{rs} + \tfrac{1}{2}S_{jk}^{\ \ i\ rs}E_i^{\ jk}. \tag{B5}$$

The requirement that the H^{rs} satisfy the commutation relations (B2) yields the system of linear equations

$$\begin{aligned}
&\eta^{ri}S_{jk}^{\ \ s\ ab} - \eta^{si}S_{jk}^{\ \ r\ ab} - \eta^{ai}S_{jk}^{\ \ b\ rs} + \eta^{bi}S_{jk}^{\ \ a\ rs} \\
&\quad - \delta_j^s\eta^{rm}S_{mk}^{\ \ i\ ab} + \delta_j^r\eta^{sm}S_{mk}^{\ \ i\ ab} + \delta_j^b\eta^{am}S_{mk}^{\ \ i\ rs} \\
&\quad - \delta_j^a\eta^{bm}S_{mk}^{\ \ i\ rs} - \delta_k^s\eta^{rm}S_{jm}^{\ \ i\ ab} + \delta_k^r\eta^{sm}S_{jm}^{\ \ i\ ab} \\
&\quad + \delta_k^b\eta^{am}S_{jm}^{\ \ i\ rs} - \delta_k^a\eta^{bm}S_{jm}^{\ \ i\ rs} \\
&= -\eta^{ra}S_{jk}^{\ \ i\ sb} - \eta^{sb}S_{jk}^{\ \ i\ ra} + \eta^{rb}S_{jk}^{\ \ i\ sa} + \eta^{sa}S_{jk}^{\ \ i\ rb}.
\end{aligned} \tag{B6}$$

The objective is to find the general solution of this linear, homogeneous system of equations.

Define

$$R_{jk}^{\ \ i} = \eta_{pq}S_{jk}^{\ \ p\ qi} = R_{kj}^{\ \ i} \tag{B7}$$

and

$$V_k = R_{mk}^{\ \ m}, \quad V^k = \eta^{km}V_m, \tag{B8}$$

and

$$H^i = \eta^{mp}R_{mp}^{\ \ i}, \quad H_i = \eta_{il}H^l. \tag{B9}$$

Then define $\hat{R}_{jk}^{\ \ i}$ by

$$\begin{aligned}
R_{jk}^{\ \ i} = \hat{R}_{jk}^{\ \ i} &+ \frac{n}{(n-1)(n+2)}\left[\delta_j^iV_k + \delta_k^iV_j - (2/n)\eta_{jk}V^i\right] \\
&- \frac{1}{(n-1)(n+2)}\left[\delta_j^iH_k + \delta_k^iH_j - (n+1)\eta_{jk}H^i\right].
\end{aligned} \tag{B10}$$

Then both the horizontal and the vertical trace of $\hat{R}_{jk}^{\ \ i}$ vanish. Also, define

$$S_k^{\ ab} = S_{mk}^{\ \ m\ ab}, \quad S^b = S_{ml}^{\ \ m\ lb} = S_l^{\ lb}. \tag{B11}$$

By contraction on r and i, (B6) yields

$$\begin{aligned}
(n-1)&S_{jk}^{\ \ s\ ab} + \eta_{jl}\eta^{sm}S_{mk}^{\ \ l\ ab} + \eta_{kl}\eta^{sm}S_{mj}^{\ \ l\ ab} \\
&= \eta^{sa}R_{jk}^{\ \ b} - \eta^{sb}R_{jk}^{\ \ a} + \delta_j^sS_k^{\ ab} + \delta_k^sS_j^{\ ab} \\
&\quad + \delta_j^a\eta^{bl}R_{lk}^{\ \ s} - \delta_j^b\eta^{al}R_{lk}^{\ \ s} + \delta_k^a\eta^{bl}R_{lj}^{\ \ s} - \delta_k^b\eta^{al}R_{lj}^{\ \ s}.
\end{aligned} \tag{B12}$$

A contraction on s and a in (B12) gives

$$\begin{aligned}
&\eta_{jl}S_{km}^{\ \ l\ bm} + \eta_{kl}S_{jm}^{\ \ l\ bm} + \eta_{jl}S_k^{\ lb} \\
&\quad = \delta_j^bV_k + \delta_k^bV_j - \eta_{jl}\eta^{bm}R_{mk}^{\ \ l} - \eta_{kl}\eta^{bm}R_{mj}^{\ \ l}.
\end{aligned} \tag{B13}$$

From (B13), it follows by contraction on j and b that

$$S^k = H^k - (n-1)V^k. \tag{B14}$$

A double contraction of (B6) on i and j and on r and k yields

$$(n-1)S_s^{\ ab} = \delta_s^aS^b - \delta_s^bS^a. \tag{B15}$$

Together, (B14) and (B15) give

$$S_k^{\ ab} = [1/(n-1)](\delta_k^aH^b - \delta_k^bH^a) - (\delta_k^aV^b - \delta_k^bV^a). \tag{B16}$$

Next, define

$$S_{ijk}^{\ \ ab} = \eta_{il}S_{jk}^{\ \ l\ ab}. \tag{B17}$$

Then (B12) becomes

$$(n-1)S_{ijk}^{\ \ ab} + S_{jki}^{\ \ ab} + S_{kij}^{\ \ ab} = Q_{ijk}^{\ \ ab}, \tag{B18}$$

where

$$\begin{aligned}
Q_{ijk}^{\ \ ab} &= \delta_i^aR_{jk}^{\ \ b} - \delta_i^bR_{jk}^{\ \ a} + \delta_j^a\eta_{il}\eta^{bm}R_{mk}^{\ \ l} - \delta_j^b\eta_{il}\eta^{am}R_{mk}^{\ \ l} + \delta_k^a\eta_{il}\eta^{bm}R_{mj}^{\ \ l} - \delta_k^b\eta_{il}\eta^{am}R_{mj}^{\ \ l} \\
&\quad + [1/(n-1)][\eta_{ij}(\delta_k^aH^b - \delta_k^bH^a) + \eta_{ik}(\delta_j^aH^b - \delta_j^bH^a)] - [\eta_{ij}(\delta_k^aV^b - \delta_k^bV^a) + \eta_{ik}(\delta_j^aV^b - \delta_k^bV^a)].
\end{aligned} \tag{B19}$$

By cyclic permutation of the indices i, j, and k, a system of three equations for the "three" unknowns $S_{ijk}^{\ \ ab}$, $S_{jki}^{\ \ ab}$, and $S_{kij}^{\ \ ab}$ is obtained, which may be solved to yield

$$S_{ijk}^{\ \ ab} = \frac{n}{(n+1)(n-2)}\left[Q_{ijk}^{\ \ ab} - \frac{1}{n}(Q_{jki}^{\ \ ab} + Q_{kij}^{\ \ ab})\right]. \tag{B20}$$

Substitution of (B10) into (B19) gives

$$Q_{ijk}{}^{ab} = \delta_i^a \hat{R}_{jk}{}^b - \delta_i^b \hat{R}_{jk}{}^a + \delta_j^a \eta_{il}\eta^{bm} \hat{R}_{mk}{}^l - \delta_j^b \eta_{il}\eta^{am} \hat{R}_{mk}{}^l + \delta_k^a \eta_{il}\eta^{bm} \hat{R}_{mj}{}^l - \delta_k^b \eta_{il}\eta^{am} \hat{R}_{mj}{}^l$$
$$+ \frac{(n+1)}{(n-1)(n+2)} [\eta_{ij}(\delta_k^a H^b - \delta_k^b H^a) + \eta_{ik}(\delta_j^a H^b - \delta_j^b H^a) + \eta_{jk}(\delta_i^a H^b - \delta_i^b H^a)]$$
$$- \frac{1}{(n-1)(n+2)} [(n^2-2)\eta_{ij}(\delta_k^a V^b - \delta_k^b V^a) + (n^2-2)\eta_{ik}(\delta_j^a V^b - \delta_j^b V^a)$$
$$+ 2\eta_{jk}(\delta_i^a V^b - \delta_i^b V^a)] . \tag{B21}$$

If the factor $n/(n+1)(n-2)$ is absorbed into $R_{jk}^{\ i}$, then

$$S_{jk}^{\ i\ ab} = \eta^{ia} \hat{R}_{jk}{}^b - \eta^{ib} \hat{R}_{jk}{}^a + (\delta_j^a \eta^{bm} - \delta_j^b \eta^{am}) \hat{R}_{mk}{}^i + (\delta_k^a \eta^{bm} - \delta_k^b \eta^{am}) \hat{R}_{mj}{}^i - (1/n)$$
$$\times [\eta^{im}(\delta_j^a \hat{R}_{mk}{}^b - \delta_j^b \hat{R}_{mk}{}^a + \delta_k^a \hat{R}_{mj}{}^b - \delta_k^b \hat{R}_{mj}{}^a) + \eta^{ip}\{\eta_{jl}(\delta_k^a \eta^{bm} - \delta_k^b \eta^{am}) + \eta_{kl}(\delta_j^a \eta^{bm} - \delta_j^b \eta^{am})\} \hat{R}_{mp}{}^l$$
$$+ (\eta^{ia}\eta^{bm} - \eta^{ib}\eta^{am})(\eta_{jl} \hat{R}_{mk}{}^l + \eta_{kl} \hat{R}_{mj}{}^l)] + \frac{(n+1)(n-2)}{n(n-1)(n+2)} [\delta_j^i(\delta_k^a H^b - \delta_k^b H^a)$$
$$+ \delta_k^i(\delta_j^a H^b - \delta_j^b H^a) + \eta_{jk}(\eta^{ia} H^b - \eta^{ib} H^a)] - \frac{(n+1)(n-2)}{(n-1)(n+2)} \left[\delta_j^i(\delta_k^a V^b - \delta_k^b V^a)\right.$$
$$\left. + \delta_k^i(\delta_j^a V^b - \delta_j^b V^a) - \frac{2}{n} \eta_{jk}(\eta^{ia} V^b - \eta^{ib} V^a)\right] . \tag{B22}$$

Provided that the factor absorbed into $R_{jk}^{\ i}$ is allowed for, this result is compatible with the definitions (B7) and (B10).

The above derivation shows that any solution of (B6) must have the form (B22). That (B22) is the general solution of (B6) may be proved by direct substitution. It is worth noting that the H^i terms, the V^i terms, the $\hat{R}_{jk}^{\ i}$ terms with the factor $1/n$ and the $\hat{R}_{jk}^{\ i}$ terms without the factor $1/n$ separately satisfy (B6).

The solution (B22) is not valid for $n = 2$ because of the factor $(n-2)$ in the denominator of (B20). However, for $n = 2$ it is readily verified that

$$Q_{jk}^{\ i\ 01} = -Q_{jk}^{\ i\ 10} = R_{jk}^{\ i} \tag{B23}$$

is the solution of (B6).

APPENDIX C: $\hat{F}_{jk}^{i}$ FOR A DIRECTING FIELD MICROSYMMETRY

In this appendix, it is shown that the traceless part $\hat{F}_{jk}^{i}$ of the second-order part F_{jk}^{i} of an infinitesimal microsymmetry of a directing field Ξ is determined by Ξ and the first-order part F_j^i of the microsymmetry.

By virtue of Theorem 5.1 and the accompanying remark, condition (5.2) gives

$$\hat{F}_{\rho\sigma}^{\alpha} \xi_1^{\rho} \xi_1^{\sigma} + 2\hat{F}_{n\rho}^{\alpha} \xi_1^{\rho} + \hat{F}_{nn}^{\alpha} - \xi_1^{\alpha}$$
$$\times [\hat{F}_{\rho\sigma}^{n} \xi_1^{\rho} \xi_1^{\sigma} + 2\hat{F}_{n\rho}^{n} \xi_1^{\rho} + \hat{F}_{nn}^{n}] = E^{\alpha}(\xi_1^{\alpha}) , \tag{C1}$$

where $E^{\alpha}(\xi_1^{\alpha})$ is the left side of (5.2). By differentiating (C1) with respect to ξ_1^{α} repeatedly and then setting $\xi_1^{\alpha} = 0$, one obtains

$$\hat{F}_{nn}^{\alpha} = E^{\alpha}(0) , \tag{C2a}$$
$$2\hat{F}_{n\beta}^{\alpha} - \delta_{\beta}^{\alpha} \hat{F}_{nn}^{n} = E_{,\beta}^{\alpha}(0) , \tag{C2b}$$
$$\hat{F}_{\beta\gamma}^{\alpha} - \delta_{\beta}^{\alpha} \hat{F}_{n\gamma}^{n} - \delta_{\gamma}^{\alpha} \hat{F}_{n\beta}^{n} = \tfrac{1}{2} E_{,\beta\alpha}^{\alpha}(0) , \tag{C2c}$$
$$\delta_{\beta}^{\alpha} \hat{F}_{\gamma\delta}^{n} + \delta_{\gamma}^{\alpha} \hat{F}_{\delta\beta}^{n} + \delta_{\delta}^{\alpha} \hat{F}_{\beta\gamma}^{n} = -\tfrac{1}{2} E_{,\beta\gamma\delta}^{\alpha}(0) . \tag{C2d}$$

From (C2b), it follows that

$$\hat{F}_{nn}^{n} = -[1/(n+1)] E_{,\rho}^{\rho}(0) , \tag{C3}$$
$$\hat{F}_{n\beta}^{\alpha} = \tfrac{1}{2}(E_{,\beta}^{\alpha}(0) - [\delta_{\beta}^{\alpha}/(n+1)] E_{,\rho}^{\rho}(0)) .$$

Similarly, (C2c) gives

$$\hat{F}_{\beta n}^{n} = -\tfrac{1}{2}[1/(n+1)] E_{,\beta\rho}^{\rho}(0) , \tag{C4}$$
$$\hat{F}_{\beta\gamma}^{\alpha} = \frac{1}{2}\left[E_{,\beta\gamma}^{\alpha}(0) - \frac{1}{n+1}(\delta_{\beta}^{\alpha} E_{,\gamma\rho}^{\rho}(0) + \delta_{\gamma}^{\alpha} E_{,\beta\rho}^{\rho}(0))\right]$$

and (C4) gives

$$\hat{F}_{\beta\gamma}^{n} = -\tfrac{1}{2}[1/(n+1)] E_{,\beta\gamma\rho}^{\rho}(0) . \tag{C5}$$

Since $E^{\alpha}(\xi_1^{\alpha})$ is determined by ξ_1^{α}, F_j^i, and the field Ξ, it follows that the $\hat{F}_{jk}^{i}$ are determined by the F_j^i and the field Ξ.

[1]Our brief remarks on the problem of motion serve to place our present work in context. We have given a thorough analysis of the historical and philosophical aspects of this problem in R. A. Coleman and H. Korte, "A Realist Field Ontology of The Causal-Inertial Structure (The Refutation of Geometric Conventionalism)," University of Regina Preprint 1981, extended version 1984, 192 pp.

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[5]See Part II of Ref. 1.

[6]See p. 173 of Ref. 1.

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[12]See p. 160 of Ref. 1.

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[15]See Ref. 4 for a detailed treatment of curve and path structures.
[16]An acceleration field is also called a spray. See Appendix A, p. 418 of W. Greub, S. Halperin, and R. Vanstone, *Connections, Curvature and Cohomology* (Academic, New York, 1972), Vol. *I*.
[17]An acceleration field which satisfies the condition (3.12) has been called an *affine* spray in Ref. 16; however, this terminology is misleading since an affine spray need not be an affine structure.
[18]S. Sternberg, *Lectures on Differential Geometry* (Prentice-Hall, Englewood Cliffs, NJ, 1965), p. 15, Theorem 4.2.
[19]R. Abraham and J. E. Marsden, *Foundations of Mechanics* (Benjamin/Cummings, Reading, MA 1978), p. 225. There is a tendency to assume that the acceleration field or spray is at least C^2 in the velocity variables.
[20]The proper time is generally used as parameter. Then $g_{rs}\gamma_1^r\gamma_1^s = 1$, and the fact that $A^i_2(\gamma_1^i)$ is not C^2 in the variables γ_1^i is masked; however, then the γ_1^i are not independent, and it is not permissible to set $\gamma_1^i = 0$ for all i.
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[25]See Sec. 5 of Ref. 4.
[26]See Theorem 2 of Ref. 4.
[27]See Sec. 8 of Ref. 11.
[28]The type of subspace structure depends on the timelike, lightlike, or spacelike nature of the covector field w_k; that is, it depends on whether the group SO(1,3) reduces to SO(3), E(2), or SO(1,2).
[29]See Appendix C of Ref. 11.

Axially symmetric gravitational radiation from isolated sources

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(Received 2 August 1983; accepted for publication 25 April 1984)

Asymptotically flat, dynamic, axially symmetric space-times are considered from the point of view of the characteristic initial value problem and the expansion of solutions in powers of r^{-1}. Imposing conditions such that the system initially be exactly static and nonradiative finally, a news function is constructed which governs the dynamics of such a space-time and which yields a finite, nonvanishing total loss of the Bondi mass. Furthermore, the Riemann tensor (to order r^{-3}) is known explicitly for all time since an expression for the mass aspect is also determined. It is also shown that the total change in the asymptotic shear is related to the total change in the Bondi mass. Finally the implications concerning transitions between two exactly stationary states are discussed.

PACS numbers: 04.30. + x, 02.40. + m

I. INTRODUCTION

The gravitational radiation emitted from an isolated source distribution in general relativity has been one of the most elusive of physical phenomena. This is true not only from the point of view of the experimentalists, who during the past two decades have been assembling sensitive devices which might eventually measure the minute changes in space-time due to the motions of astrophysical objects, but also from the point of view of the theoreticians, who during a period lasting over three times as long have searched for an equally evasive result: a means by which one could determine a solution to the Einstein field equations which would represent a dynamic, asymptotically flat space-time. Such a system is normally thought of as one for which there exists a body or a collection of bodies that are confined within a world tube of compact space-like extension for all time.

Since, due to the complicated nature of the nonlinearities presented by Einstein's equations, it is highly unlikely that an exact time-dependent, asymptotically flat solution will be obtained in the near future, a number of methods have been developed which treat different aspects of the field equations to varying degrees of approximation. Perturbation procedures which date from the inception of general relativity and the first attempts to make conclusions concerning gravitational radiation have evolved to an outstanding level of sophistication. Yet in spite of the intriguing mathematical paraphernalia that has been introduced, such as matched asymptotic expansions, regularization of point masses, curved-space wave operators, etc., a number of criticisms are waged against the validity of such approximation methods. For example, the assurance is still lacking that the techniques using successive iterations, which are presently of a purely formal nature, do in fact produce expressions that converge to exact solutions of the field equations. Perturbation calculations also rely upon expansions in terms of parameters whose values must be considered to be small in comparison to unity. As is often the case, interesting relativistic effects become dominant when the values of these parameters are nearly equal to 1. In situations where one cannot postulate a small expansion parameter other methods of obtaining solutions must be employed. Often the validity of the perturbation method is called into question since one cannot make precise statements concerning the errors associated with the higher-order terms neglected in the approximation procedures.

During the past twenty years or so, the description of gravitational radiation and asymptotic flatness based upon the analysis of the null or characteristic surfaces of a space-time has led to a great understanding of the properties of the gravitational field in regions where the space-time closely resembles that of Minkowski space. While this method, first introduced by Bondi and his collaborators,[1] has blossomed into a full-fledged and usefully descriptive theory, it avoids the difficulties associated with a description of the region immediately surrounding the sources of the gravitational field, where a host of unknown nonlinear effects are likely to occur.

More recently numerical calculations performed on large-scale computers have been added to the armament of methods created to deal with the theoretical problems that must be overcome in order to gain a more complete understanding of the properties of gravitational radiation. The goals in this domain are by far the most ambitious since an "exact" description of both the behavior of the gravitational field and its sources is sought. However, still being in its infancy, many technical difficulties remain to be resolved before an unambiguous solution to the problems occurring in dynamic strong field, fast motion relativity is provided for by this method.

From the point of view of the experimentalist who will eventually make a direct measurement of the changes in gravitational curvature due to the propagation of disturbances emanating from a bounded source distribution, asymptotic procedures may not simply be last resort techniques to be applied in view of the lack of knowledge of general methods for determining dynamic solutions to the Einstein equations.

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 0022-2488/84/123527-11$02.50

Since a gravitational wave detector will most likely be located at astronomical distances from any realistic emitter, the properties associated with the behavior of material sources will eventually have to be deduced from direct measurements of the asymptotic Riemann tensor components. The measurements must therefore be correlated with what can be known theoretically about the asymptotic Riemann tensor. Whether or not the remote observer will ever, by purely gravitational measurements alone, be able to distinguish between radiation emitted from concentrations of gravitational curvature and compact distributions of matter has been called into question recently by the work of Lawitzky[2] who has demonstrated that dynamic exterior gravitational fields may have vacuum sources as well as different sources consisting of matter distributions.

Asymptotics also have certain theoretical advantages. The first being that unambiguous definitions of such notions as energy loss, incoming radiation, stationarity, etc., can be introduced. Second, it has been demonstrated that if the reduced analytic initial data obey certain conditions, then the Bondi type expansions are in fact convergent to solutions of the Einstein equations.[3] These methods can therefore offer an exact description of the behavior of the gravitational field far from an isolated source distribution.

The purpose of this paper then is to analyze the characteristic initial value problem with a view toward obtaining explicit expressions which might lead to a convergent asymptotic series solution to Einstein's equations and from which the exact asymptotic properties of the Riemann tensor may be discussed. In particular, the construction of a space-time which is permanently isolated and demonstrates certain physically reasonable behavior is considered. This task is quite formidable in its completely general form where there exist no Killing vector fields. Therefore, certain symmetry requirements will be imposed in order to simplify the field equations. However, the "highest" symmetry that permits gravitational radiation from a permanently isolated system is that of axial symmetry with one hypersurface orthogonal (rotational) Killing vector field. The imposition of any additional symmetries yields solutions which if permanently isolated are static and therefore nonradiative, or, if radiative, are not always confined to a limited three-dimensional region of spatial extent. These latter solutions include the plane and cylindrical wave solutions as well as the boost-rotation symmetric solutions.[4]

Therefore, the next section introduces a mathematical description of axially symmetric space-times convenient for the discussion of systems that undergo gravitational transitions from one nonradiative state to another nonradiative state. After a brief review of previous attempts to understand the nature of permanently isolated dynamic axisymmetric systems, a method is presented in Sec. III that leads to the construction of a news function which yields a nonzero, finite mass loss associated with a system having no incoming radiation. Section IV is devoted to a discussion of some of the general properties of the news function as well as the higher-order Bondi functions. Finally this paper concludes with some observations concerning the advantages and disadvantages of the asymptotic techniques.

II. AXIALLY SYMMETRIC SPACE-TIMES: AN ASYMPTOTIC DESCRIPTION

A. General considerations

The analysis of the asymptotic behavior of the gravitational field associated with an insular radiating source distribution commences with the formalism introduced by Bondi, van der Berg, and Metzner[1] who, using a suitably chosen coordinate system, were able to investigate the properties of the solutions of the Einstein field equations corresponding to axially symmetric isolated systems. Such space times with circular group orbits admit a hypersurface orthogonal Killing vector field that will be denoted by $\partial/\partial\phi$. In order to describe the emission of gravitational waves, the coordinate variables are given as $\{x^0, x^1, x^2, x^3\} = \{u, r, \theta, \phi\}$, where θ and ϕ are the polar and azimuthal angles, respectively, and u is the retarded time, labeling outgoing light cones, which is constant together with θ and ϕ along a null geodesic. The radial coordinate r is chosen to be the luminosity distance, defined in such a manner that the area of the surfaces with constant r and u is equal to $4\pi r^2$. In this coordinate system, the line element satisfying the vacuum field equations takes the following form:

$$ds^2 = (V e^{2\beta}/r)\,du^2 + 2\,e^{2\beta}\,du\,dr - r^2\,[e^{2\gamma}(d\theta - U\,du)^2 + e^{-2\gamma}\sin^2\theta\,d\phi^2]. \quad (2.1)$$

The metric functions, V, U, β, and γ are functions of the coordinate variables r, u, and θ and the condition that the solution be truly isolated requires that the functions be regular everywhere; in particular on the polar axis ($\theta = 0, \pi$), i.e.,

$$V,\ \beta,\ (U/\sin\theta), \text{ and } (\gamma/\sin^2\theta) \quad (2.2)$$

are regular functions of $\cos\theta$ at $\cos\theta = \pm 1$.

The known solutions of the field equations which exist and obey the regularity conditions are the static, asymptotically flat, Weyl class of solutions. Known radiative solutions which can be explicitly given in terms of analytic functions are singular on the axis of symmetry and therefore cannot be considered as representing truly isolated systems. The best examples of exact solutions which represent radiative systems with known sources are the boost-rotation symmetric solutions,[4] which include the Bonnor–Swaminarayan solution[5] and the C-metric.[6] Physically speaking, the extra boost symmetry requires that the sources undergo uniformly accelerated motion along the polar axis. This may result, for example, from introducing stresses which extend to infinity along the axis or from locating an infinitely large mass infinitely far away. Uniform acceleration is clearly an unphysical situation if it exists for all time. Hence solutions of such a nature are not considered to be permanently isolated. Therefore, in what follows, it will be required that the conditions (2.2) must be satisfied for all retarded times u.

Even for the case of axial symmetry, the field equations are extremely complicated, and since no exact time-dependent asymptotically flat solutions are known, one assumes that the metric functions may be expanded in terms of a series in powers of r^{-1} and the vacuum field equations are then employed to determine the precise form of the development in terms of certain functions of integration:

$$\gamma = c(u,\theta)\,r^{-1} + [C(u,\theta) - \tfrac{1}{6}c^3]\,r^{-3} + G(u,\theta)\,r^{-4} + O(r^{-5}), \tag{2.3}$$

$$\beta = -\tfrac{1}{4}c^2 r^{-2} + O(r^{-4}), \tag{2.4}$$

$$U = -(c_{,2} + 2c\cot\theta)\,r^{-2} + [2N(u,\theta) + 3cc_{,2} + 4c^2\cot\theta]\,r^{-3} + O(r^{-4}), \tag{2.5}$$

$$V = r - 2M(u,\theta) + [N_{,2} + N\cot\theta - c_{,2}^2 - 4c_{,2}\,c\cot\theta - \tfrac{1}{2}c^2(1 + 8\cot^2\theta)]\,r^{-1} + O(r^{-2}), \tag{2.6}$$

and where

$$4C_{,0} = 2c^2 c_{,0} + 2cM + N\cot\theta - N_{,2}, \tag{2.7a}$$

$$-4G_{,0} = C_{,22} + C_{,2}\cot\theta + 2C(1 - 2\cot^2\theta) - 2(cN)_{,2} - 6cN\cot\theta. \tag{2.7b}$$

Here commas denote partial differentiation with respect to the appropriate coordinate variable. The three arbitrary functions of integration $c(u,\theta)$, $M(u,\theta)$, and $N(u,\theta)$ are connected by the following relations derived from the field equations:

$$M_{,0} = -c_{,0}^2 + \tfrac{1}{2}(c_{,22} + 3c_{,2}\cot\theta - 2c)_{,0}, \tag{2.8}$$

$$-3N_{,0} = M_{,2} + 3cc_{,02} + 4cc_{,0}\cot\theta + c_{,0}c_{,2}. \tag{2.9}$$

The structure of the field equations is such that the asymptotic initial value problem is posed in the following manner: it is necessary to give $r(r,\theta)$ on an outgoing null cone defined by $u = \text{const}$. Along a timelike cylinder located far from the sources (in the limit $r \to \infty$) one must give $c(u,\theta)$, and at the intersection of the light cone with the cylinder, the angular dependence of M and N is given. Since the information concerning the changes in the field is governed by $c(u,\theta)$, the name "news function" is normally given to the time derivative of this particular function. The function $c(u,\theta)$ is normally called the asymptotic shear, $M(u,\theta)$ the "mass aspect," and the other functions N,C, G, etc. will be called the "multipole aspects" for reasons which will be evident later in this discussion. Recently Friedrich[3] has demonstrated that analytic initial data posed on a light cone where u is finite does in fact lead to a convergent Bondi type expansion. Since $c(u,\theta)$ must vanish on the axis like $\sin^2\theta$, one introduces, in order to facilitate the calculations that are to follow,; the change of variable $\mu = \cos\theta$ and the function $g(u,\mu)$ defined such that

$$g(u,\mu) \equiv \frac{c(u,\theta)}{\sin^2\theta} = \frac{c(u,\mu)}{1-\mu^2}. \tag{2.10}$$

Using these definitions the "Bondi supplementary conditions" [Eqs. (2.8) and (2.9)] may be written as

$$\dot{M} = -\dot{g}^2(1-\mu^2)^2 + \tfrac{1}{2}[\dot{g}(1-\mu^2)^2]'', \tag{2.11}$$

$$3\dot{N} = (1-\mu^2)^{1/2}[M' + (3g\dot{g}' + \dot{g}g')(1-\mu^2) - 12g\dot{g}\mu(1-\mu^2)]. \tag{2.12}$$

Hereafter in this work the symbol dot ($\dot{}$) and prime ($'$) will denote partial differentiation with respect to the variables u and μ, respectively.

In general the three functions g, M, and N will depend in a rather complicated manner upon u and μ, and their physical significance will be rather obscure owing to the lack of knowledge of the behavior of the sources. However when the system is time independent, the new free Bondi metric may be compared with the asymptotically flat static solutions of the Weyl–Levi–Civita class. The only Weyl solution known to have an exact counterpart in the Bondi system is the Schwarzschild solution, the others being determined as an expansion in r^{-1} where the coefficients are given in terms of multipole moments. If m, D, Q, and P are the monopole, dipole, quadrupole, and octopole moments, respectively, of a static axially symmetric distribution of energy defined such that all multipole moments higher than monopole vanish for the Schwarzschild solution, then the relationships between the first four moments occurring in the general Weyl solution and the Bondi functions are the following:

$$\begin{aligned} &M = m, \quad N = (1-\mu^2)^{1/2}(D + mF'),\\ &C = (1-\mu^2)[\tfrac{1}{2}Q + DF' + \tfrac{1}{2}m(F')^2],\\ &\tfrac{4}{5}G = (1-\mu^2)\{(P - m^2 D)\mu + (mQ - D^2)\\ &\quad - \tfrac{1}{2}Q[F''(1-\mu^2) - 6F'\mu]\\ &\quad - F'D[F''(1-\mu^2) - 3F'\mu]\\ &\quad - \tfrac{1}{2}m(F')^2[F''(1-\mu^2) - 2F'\mu]\}, \end{aligned} \tag{2.13}$$

where $F(\mu)$ is an arbitrary function of μ. These are the most general news free static relationships that may occur. In this case g is independent of u and the asymptotic shear $g = g(\mu)$ is determined from a function $F(\mu)$ by

$$g(\mu) = -\tfrac{1}{2}F''. \tag{2.14}$$

Since the Weyl multipole moments are simply constants, (2.13) demonstrates that the "mass aspect" $M(u,\mu)$, in the static case, is independent not only of u but of μ as well; it being exactly the mass monopole term. The higher-order Bondi functions are, in the time-independent case, seen to be closely related to the respective higher-order multipole moments.

The function $F(\mu)$ expresses what is known as the supertranslation freedom that exists in defining the outgoing light cones by the parameterization u, i.e.,

$$\bar{u} = u + F(\mu). \tag{2.15}$$

The Bondi functions are determined (in the static case) exactly by the Weyl multipoles when $F(\mu) = \text{const}$. In other words a simple renumbering of the light cones does not affect the Bondi form of the Weyl metric. The condition that the static solution be free of asymptotic shear is expressed by the fact that $g(\mu)$ vanishes, in which case F is an arbitrary linear function of μ.

In the general time-dependent situation, the simple relationships (2.13) can no longer be fulfilled and one must integrate the evolution equations (2.7)–(2.9) with respect to time in order to determine the precise values of the higher-order Bondi functions. The hierarchy of these equations is such that the evolution of each multipole aspect depends only upon the lower-order functions and that a specific solution up to order r^{-n} is determined by the values that the n-pole aspects take on the initial light cone.

One now defines the Bondi mass as the average, over the sphere, of the mass aspect,

$$m(u) \equiv \frac{1}{2}\int_0^{\pi} M(u,\theta)\sin\theta\, d\theta = \frac{1}{2}\int_{-1}^{1} M(u,\mu)\, d\mu, \tag{2.16}$$

and this may be thought of as representing the total mass of the system as a function of the retarded time; an interpretation that is obvious when the system is static. Combining expression (2.16) with that of (2.11) and maintaining the regularity conditions, one obtains the well-known result that the Bondi mass is a monotonically decreasing function of the retarded time since the second term on the right-hand side of (2.11) vanishes when integrated over the sphere

$$\dot{m}(u) = -\frac{1}{2}\int_{-1}^{1} \dot{g}^2(u,\mu)(1-\mu^2)\, d\mu. \tag{2.17}$$

Since one will eventually be interested in making a measurement of the effects of the radiation emitted from a system that undergoes a loss of its Bondi mass, the expressions for the asymptotic Riemann tensor components must be calculated. Once again employing the $1/r$ expansion, the nonvanishing components (to order r^{-3}) are found to be

$$\begin{aligned}
R_{0022} &= -R_{0033} = -R_{0122} = R_{0133} = R_{1122} = -R_{1133} \\
&= -\ddot{g}(1-\mu^2)\, r^{-1} + (\tfrac{1}{2}\dot{g}''(1-\mu^2)^{1/2} \\
&\quad - 3\dot{g}'\mu - 2\dot{g})(1-\mu^2)\, r^{-2} + \cdots, \\
R_{0012} &= -R_{1021} = -R_{0233} = R_{1233} \\
&= (1-\mu^2)^{1/2}[\,\dot{g}'(1-\mu^2) - 4\dot{g}\mu\,]\, r^{-2} + \cdots, \\
R_{0011} &= -R_{2233} = -2(M + g\dot{g}(1-\mu^2)^2)\, r^{-3} + \cdots .
\end{aligned} \tag{2.18}$$

In this paper, the point of view will be taken that the presence of nonzero coefficients appearing in the r^{-1} and r^{-2} terms of the Riemann tensor are indications of radiative and quasiradiative behavior, respectively.Therefore while $\dot{g} \neq 0$ expresses the fact that the mass aspect is undergoing a change, $\ddot{g} \neq 0$ states that the Riemann tensor is able to measure the presence of radiation.

B. Axially symmetric pulsed radiation

Suppose now that there exists a system which exhibits some radiative behavior in the time interval $u_0 < u < u_1$. During this period of time it will be assumed that there is a change in the mass aspect which requires also that the news function be nonvanishing. At retarded times $u \leqslant u_0$ it will be assumed that the system is nonradiative; a situation which must be distinguished from one that is truly static. When a system is in a nonradiative state, it will be assumed that following conditions hold:

$$\ddot{g}(u,\mu) = \dot{g}(u,\mu) = \dot{M}(u,\mu) = 0. \tag{2.19}$$

A truly static state on the other hand requires that not only are all of the Bondi functions independent of the time variable but that their angular dependence take on exactly the dependence given by comparison with the Weyl metric, i.e., Eqs. (2.13). The physical interpretation of systems that are nonstatic and nonradiative is a major outstanding problem. Though a system may have $\dot{M} = 0$, that is not enough to guarantee that N, C, G, and the other high-order functions be independent of u. A simple example (given originally by Bondi *et al.*) is a situation where a Schwarzschild mass moves with constant velocity along the axis of symmetry. In such a case N varies linearly with u, C is a quadratic function of u and all higher-order functions are also dependent upon u. Other uncommon situations can exist such as a system that is initially radiative without a mass loss [e.g., when $u = u_0 = 0$ and $g(u,\mu) = f(\mu)\, u^2$]. Such systems still present problems concerning their physical interpretations. Commencing with a static Weyl solution at $u = u_0$ has the advantage that one is certain that the Bondi expansion is truly convergent prior to the moment at which the dynamic behavior commences and that there are no ambiguities surrounding the physical interpretation of the nonradiative state. However this requirement may be in fact too restrictive and may not be able to describe a large number of interesting physical situations.

If a pulse of radiation is to be produced, then for retarded times later than u_1 conditions (2.19) must once again hold. In addition the imposition that the final state be static requires that one integrate the evolution equations over the period of radiative behavior and that the final multipole aspects in fact have the Weyl angular dependence. Since there are an infinite number of these equations and there exist no conservation laws for the coefficients appearing in the expansion of γ beyond the r^{-4} term,[7] it then seems quite improbable that a news function can be constructed which governs the evolution between two exactly static states.

Outside of the supertranslation freedom that one has in choosing the enumeration of the outgoing light cones, there exists also the freedom of performing conformal transformations of the sphere to itself, i.e., that lengths can undergo a conformal rescaling

$$d\tilde{u} = K\, du,$$

which is equivalent to performing a Lorentz transformation where the system is given a constant velocity v, directed along the axis of symmetry. In this case $K = x^{-1}(1 + v\mu)$, where $x = (1-v^2)^{1/2}$, and the once static Bondi functions defined by choosing a particular $F(\mu)$ become

$$\begin{aligned}
\tilde{g} &= xg(1+v\mu)^{-1} = -\tfrac{1}{2}xF''(\mu)(1+v\mu)^{-1}, \\
\tilde{M} &= mx^3(1+v\mu)^{-3}, \\
\tilde{N} &= \frac{(1+\mu^2)^{1/2}}{(1+v\mu)^3}\, x^3\left(D + mF' - \frac{mvu}{1+v\mu}\right).
\end{aligned} \tag{2.20}$$

In this case one can easily interpret a particular nonstatic, nonradiative situation: that for which a nondynamic system moves with constant velocity along the polar axis. Clearly the angular dependence of M is not the Weyl dependence and integration of (2.12) yields a linear time dependence for N which in turn would lead to a quadratic time dependence for $C(u,\mu)$, etc. More general cases have been discussed by Bondi *et al.*[1] and Bonnor and Rotenberg[8] where the first few Bondi functions do in fact obey the Weyl conditions initially and finally, but where at some higher order the functions exhibit a time dependence. How one would distinguish between fields which represent radiative "tails" or radiation reaction forces acting upon the higher-order multipoles without information concerning the actual source behavior

is in itself a very difficult question and, as yet, remains unanswered.

In order that one maintain a certain ability to give a physical interpretation to the behavior of the gravitational field far from the source, the conformal factor K will be chosen such that initially the mass aspect is given by the mass monopole and is therefore independent of u and μ. Since the initial data may be freely given, it will be assumed that the initial state of the system is exactly static and that all of the remaining Bondi functions take on their Weyl values. Therefore the frame is fixed to be comoving with the initially static state, i.e., $v_{\text{initial}} = 0$.

After the pulse of radiation has occurred, the mass monopole part may be left with a finite velocity v_f with respect to the frame fixed to the initially static configuration. In this case the total change in the mass aspect will be given by

$$\Delta M_{\text{total}} = m(u_1)(1 - v_f^2)^{3/2}(1 + v_f \mu)^{-3} - m(u_0). \quad (2.21)$$

A very special situation would be that for which no "total radiation reaction force" occurs and the final expression for the mass aspect is also independent of μ. In that case the total change in the mass aspect is equal to the total change in the Bondi mass

$$\Delta M_{\text{total}} = \Delta m_{\text{total}} \quad (2.22)$$

and integrating Eqs. (2.11) and (2.17) throughout the interval during which the radiative behavior occurs yields the following relationship:

$$-\int_{u_0}^{u_1} \dot{g}^2\, du(1-\mu^2)^2 + \frac{1}{2}\left[(g(u_1) - g(u_0))(1-\mu^2)^2\right]'' = -\frac{1}{2}\int_{-1}^{1}\int_{u_0}^{u_1} \dot{g}^2(1-\mu^2)^2\, du\, d\mu. \quad (2.23)$$

It is this equation which will be used for the remainder of this paper in order to determine an expression for $g(u, \mu)$ that will serve as the starting point for constructing a space-time which should yield a description of the gravitational radiation emitted from a permanently isolated system.

III. CONSTRUCTION OF THE NEWS FUNCTION

The problem of constructing an axially symmetric space-time that is truly isolated and, hopefully, significant physically resides in the determination of a function $g(u, \mu)$ which is regular and governs the dynamic evolution between two nonradiative states that has associated with it a finite loss of the Bondi mass. While $g(u, \mu)$ represents the part of the data which is freely specifiable, a random choice for this function normally leads to changes in the mass aspect that defy any physically significant interpretation. Even if one imposes the restrictions (2.19) there exist still many choices for $g(u, \mu)$, but the regularity conditions along with the condition that the transition obey Eq. (2.23) seem to place severe restrictions on $g(u, \mu)$, so much so that there has been a rather long history of failed attempts to construct such a news function. The fact that a finite mass loss seems to imply some sort of physically realizable system has been perhaps the greatest motivation behind such attempts.

Before discussing how one may in fact construct such an expression for $g(u, \mu)$, a brief review of the methods which have already been employed previously is perhaps in order. Historically, the first attempts to construct an axisymmetric news function obeying Eq. (2.22) appeared in the original paper by Bondi *et al.*,[1] where the general form

$$\dot{g}(u, \mu) = \sum_{n=0}^{\infty} f_n(\mu)\, h_n(u) \quad (3.1)$$

was employed. Expressions for $f_n(\mu)$ and $h_n(u)$ were found only to order $n = 2$ after which the equations became too unwieldly to handle comfortably. Next Bonner and Rotenberg[8] using a double series expansion, tried constructing an expression similar to (3.1). They analyzed a system which, to the order considered, initially could be described by a Schwarzschild solution with $g = 0$ and, which after undergoing a period of radiative behavior became another Schwarzschild solution (again with $g = 0$) though the final mass was found to undergo a finite constant velocity motion due to "radiation reaction." As in the Bondi attempt only terms to the second order were considered since the equations quickly became very complicated with increasingly higher iterations.

Employing the fact that the boost-rotation symmetric solutions could be considered as radiating systems, Bicak[5] who analyzed the Bonner–Swaminarayan solution and Kinnersley and Walker[6] who analyzed the C-metric used asymptotic methods for determining certain radiative properties. More recently[4] it has been shown that a generalization of these metrics yields a news function which takes on the form

$$\dot{g}(u, \mu) = H\,(u_f/(1-\mu^2)^{1/2})(1-\mu^2)^{-2}, \quad (3.2)$$

where H is a general function of the argument $u_f(1-\mu^2)^{-1/2}$ and u_f is the flat space retarded time $u_f = t - r$. Though the boost-rotation symmetric solutions are the best examples of an exact radiating solution with known source distributions, the irregularity on the axis causes the Bondi mass to diverge and nothing can be said about a total mass loss since in a physical sense energy must be continuously added to the system to maintain the constant acceleration of the "particle" sources.

In order to make some link between source motions and the dynamics of the fields at null infinity the formal perturbation procedures alluded to in the Introduction have been used to determine the news function to within a certain order determined by a small expansion parameter. For problems dealing specifically with axial symmetry, D'Eath[9] analyzed the problem of a two-black-hole collision where the velocity of each was close to the velocity of light and Cooperstock and Hobill[10] analyzed the problem of a two-body collision which began from rest. The expressions for the news function in both cases however, exhibit an irregular nature on the axis of symmetry. Indeed outside of questions of convergence, the known approximation methods seem unable to provide enough information for the construction of a news function which obeys the necessary requirements that the system be perfectly isolated. Bonnor and Rotenberg had issued a warning against the use of such a technique in saying "that to start [the Bondi expansion] off one needs to have more information than is available from the linear approximation. This is because the news function which generates the solution, contains nonlinear terms which one does not

know from the start. It is therefore not clear how given a particular physical system one can put the method into operation."

Thus, while the Bondi method is attractive in that it provides "exact" information concerning a radiating system and can lead to a convergent series solution, it is not a cure for the maladies associated with the perturbation methods in current use which begin from a linearization of the field equations.

Finally mention must be made of the work of Papapetrou[11] and Hallidy and Janis[12] who consider the problem of axially symmetric transitions between two static states and the ability to remove the radiation "tails." Both considered, essentially, a function $g(u,\mu)$ given by the expansion

$$g(u,\mu)=\sum_{l=2} a_l(u)[P_l(\mu)]'', \tag{3.3}$$

where the coefficients $a_l(u)$ are functions of u in the general case and reduce to constants when the system is static. The functions $P_l(\mu)$ are the Legendre polynomials. It was demonstrated in both papers that no possible solutions could exist which both satisfied (2.22) and had a finite number of terms in the expansion. One could not therefore arrive at any news function giving a finite mass loss by truncating the expression (3.3). If a transition betwen two static states was required then a closed form expression for $g(u,\mu)$ would be needed, should one exist.

With these previous attempts in mind, and since there are no general techniques by which one may find solutions to an equation such as (2.23), one must resort to a method where a particular form for the time dependence of $g(u,\mu)$ is assumed together with a number of arbitrary functions of μ that are to be determined from evaluating the left-hand side of (2.23) and from applying the regularity conditions. The regularity of $g(u,\mu)$ is important as it allows an unambiguous determination of the total mass loss. Since $M(u,\mu)$ is assumed to be independent of u and μ both initially and finally, an evaluation of its total change on any generator of null infinity, i.e., for any $\mu=$ const in this case, will yield the same expression for the total change of the Bondi mass. Expanding the second term on the left-hand side of Eq. (2.23) yields

$$\int_{u_0}^{u_1}\dot{g}^2\,du(1-\mu^2)^2+\frac{1}{2}(\Delta g)''(1-\mu^2)^2-4(\Delta g)'(1-\mu^2)\mu + 2(3\mu^2-1)(\Delta g)=\Delta M_{\text{total}}. \tag{3.4}$$

Evaluating this expression on the axis at $\mu=\pm 1$ yields a very simple expression for the total mass loss,

$$\Delta m_{\text{total}}=4[\,g(u_1,\mu=\pm 1)-g(u_0,\mu=\pm 1)], \tag{3.5}$$

and one has that, on the axis, the initial and final values of the function $g(u,\mu)$ must differ in order to give a nonzero mass loss. Due to the fact that m is a monotonically decreasing function of retarded time, the function g must demonstrate a certain asymmetry with respect to time, i.e.,

$$g(u_0,\mu=\pm 1)>g(u_1,\mu=\pm 1), \tag{3.6}$$

which is a relationship which will hold in general (except perhaps in a few isolated directions). Using the fact that one can always, via the use of a supertranslation, put a stationary system into a coordinate frame that is shear-free, some authors have attempted to determine a news function giving an axially symmetric pulse of radiation between two static states, both of which are shear-free. If one is to use the *same* frame for the description of the complete evolution this is not at all possible. Nor can one define then a system of "good cuts" for the light cones, i.e., one obeying the equation $F''=0$; for in that case there will be no mass loss and hence no radiation.

Since the sum of the terms on the left-hand side of Eq. (2.23) must be independent of μ, the simplest choice of news function would be one which might make each term individually independent of μ. That this choice must be immediately ruled out is demonstrated by the following: suppose both terms on the lhs of (2.23) are independent of μ, then

$$\{[\,g(u_0,\mu)-g(u_1,\mu)](1-\mu^2)^2\}''=0,$$

which leads to either

(a) $g(u_0,\mu)=g(u_1,\mu)$

or

(b) $\Delta g(\mu)=(k_1\mu+k_0)/(1-\mu^2)^2$,

where k_0 and k_1 are constants.

The requirement that the mass loss be nonzero rules out (a) while the regularity conditions are in contradiction to (b). Therefore in order that the two terms on the lhs of Eq. (2.23) yield an expression independent of μ, the dependence of $g(u,\mu)$ on μ must be of a more complicated nature.

The assumption that the solution initially be exactly a Weyl solution requires not only that the conditions (2.19) hold but also that the time derivatives of all orders of $g(u,\mu)$ vanish at u_0 and therefore the time-dependent functions appearing in the asymptotic shear must be of class C^∞. This has the effect of pushing the initial light cone $u=u_0$ to the limit $u_0\to-\infty$ and the initial static state is an asymptotic state in the infinite past, otherwise a system which is truly static up to a finite time must have discontinuous time derivatives at some finite order. In a similar manner a final static state requires the vanishing of all time derivatives $g(u,\mu)$ after the period of radiative behavior, and this must occur in the infinite future. The period of radiative behavior then becomes $-\infty<u<\infty$ which puts one outside of the domain of the convergence criteria of Freidrich. In addition the values of M and N must be given at the intersection of past null infinity with future null infinity. When the mass term is nonvanishing one is confronted with the unsolved problem of being able to "connect" the two null infinities.

In spite of this important theoretical problem, it will be demonstrated that there does exist at least one expression for g whose time derivatives to all orders vanish initially and finally. This expression also yields a total change in the mass aspect which is finite and independent of the angular coordinates.

A general expression for the asymptotic shear that is able to satisfy both the requirement that

$$\lim_{u\to\pm\infty}\frac{\partial^n}{\partial u^n}g(u,\mu)=0,$$

and the inequality (3.6) is given by the rational function

$$g(u,\mu) = (f_1 e^{\eta u} + f_3)/[f_2 e^{\nu u} + f_4]^{\rho}, \tag{3.7}$$

where ρ, ν, η are rational constants obeying the relation $\eta < \nu\rho$ and $f_n(\mu)$ $(n = 1,2,3,4)$ are functions of μ to be determined by Eq. (2.23). For g to be defined everywhere, f_1 and f_2 must not vanish (or become infinite) for any value of μ. Otherwise as the exponential function becomes infinite (or vanishes) the function g becomes undefined when the limits with respect to μ and u are interchanged. Finally, one requires that the functions f_n all be real, since there do exist cases where a finite mass loss can lead to f_n's which are imaginary. This occurs, for example, when $\eta = \nu$ and $\rho \geqslant 1$.

Even at this time there still remains a large degree of arbitrariness, particularly with the choice of the constants appearing in the exponential arguments, and without any further simplification, the expression (3.7) and its first time derivative when introduced into Eq. (2.23) result in long recursion formulas involving a large amount of algebra. Therefore the following procedure will be employed: η and ν will be given a particular relationship (which in turn places limits on ρ) then Eq. (2.23) will be evaluated, and the f_n's and ρ will finally be chosen so as to satisfy the restrictions that have been already imposed on the metric functions $g(u,\mu)$ and $M(u,\mu)$.

Therefore after choosing $\nu = 2\eta$ and determining the integral $\int_{-\infty}^{\infty} \dot{g}^2\, du$ one obtains

$$\int_{-\infty}^{\infty} \dot{g}^2\, du = \eta \left\{ \frac{1}{2(2\rho+1)} \left[\frac{f_1^2}{f_2 (f_4)^{2\rho-1}} + \frac{2\rho f_3^2}{(f_4)^{2\rho}} \right] + \left[\frac{3(2\rho-1)}{(4\rho-1)} - 1 \right] \left[\frac{4\rho f_1 f_3 f_4}{(4\rho+1)} I_{2\rho+1} \right] \right\}, \tag{3.8}$$

where

$$I_{2\rho+1} = \frac{(4\rho-3)!!}{2^{2\rho+2}(2\rho+1)!(f_4)^{2\rho+1}} \frac{\pi}{\sqrt{f_2 f_4}}.$$

The choice $\rho = 1$ has a number of advantages. Firstly it eliminates the factors of π which would otherwise appear in the total mass loss, and it is the only choice for $\rho < 8$ which yields real functions of μ. Finally it simplifies many of the algebraic expressions that appear in subsequent calculations. Note that with this choice of constants, and with a proper choice of the f_n's, one can have that $g(\infty,\mu) = 0$, which permits the possibility of attaining the Schwarzschild solution as a final state should one be able to arrive at a truly static system in the infinite future. This may be seen from the fact that the Schwarzschild metric in Bondi coordinates is given by $V = r - 2m$, $U = \gamma = \beta = 0$, where m is the Schwarzschild mass parameter.

The following expression for the total mass loss can now be obtained:

$$-\Delta M = \frac{\eta}{6} \left[\frac{f_1^2}{f_2 f_4} + 2\frac{f_3^2}{f_4^2} \right] (1-\mu^2) + \frac{1}{2} \left[\frac{f_3}{f_4} (1-\mu^2)^2 \right]''. \tag{3.9}$$

Now in the limit $u \to -\infty$ the function $g \to f_3/f_4$, and by (2.2) this ratio must be a regular function of μ as $\mu \to \pm 1$. Define $A(\mu)$ as

$$A(\mu) = f_3/f_4. \tag{3.10}$$

The functions $f_1(\mu)$ and $f_2(\mu)$ as well as $A(\mu)$ must be nonzero, and from (3.10) one has that the term $(f_3/f_4)^2(1-\mu^2)^2$ is equal to the product of a regular nonzero function of μ with a fourth-order polynomial of μ. This property will also be assumed for the product of $f_1^2/(f_1 f_4)$ with $(1-\mu^2)^2$. That is,

$$(f_1^2/f_2 f_4)(1-\mu^2)^2 = B^2(\mu)(1 + k\mu + l\mu^2 + p\mu^3 + q\mu^4), \tag{3.11}$$

where the coefficient of μ^0 has been absorbed into the function $B(\mu)$ which is regular on the axis.

The expressions (3.10) and (3.11) are now inserted into (3.9) and (2.23) and one obtains the following system of equations by equating the coefficients of the various powers of μ:

$$(n/6)[qB^2 + 2A^2] + A''/2 = 0, \tag{3.12}$$

$$(\eta/6)[pB^2] + 4A' = 0, \tag{3.13}$$

$$(\eta/6)[lB^2 - 4A^2] + 6A - A'' = 0, \tag{3.14}$$

$$(\eta/6)[kB^2] - 4A' = 0, \tag{3.15}$$

$$(\eta/6)[B^2 + 2A^2] + A''/2 - 2A = \frac{1}{2}\int_{-1}^{1} \left\{ -\frac{A''}{2}\mu^4 - 4A'\mu^3 + (A'' - 6A)\mu^2 + 4A'\mu + \frac{\eta}{6}[B^2 + 2A^2] \right\} d\mu, \tag{3.16}$$

where Eqs. (3.12)–(3.15) have been used to simplify the integrand appearing in Eq. (3.16). Note that had the expression (3.11) involved a polynomial of order less than 4, then all of the numerical coefficients would vanish, thereby yielding $\Delta M = 0$.

Immediately from Eqs. (3.13) and (3.15) one obtains the relation

$$p = -k, \tag{3.17}$$

while Eqs. (3.12) and (3.14) yield

$$(\eta/6)[(2q+l)B^2] = -6A. \tag{3.18}$$

Differentiating this last equation with respect to μ gives an expression for A' which together with Eq. (3.13) yields a simple first-order differential equation for B with the solution

$$B(\mu) = m_b \exp[\tfrac{3}{4}(P/(2q+l))\mu], \tag{3.19}$$

where m_b is an arbitrary constant, that in geometric units, has units of length. From this expression and (3.19) one easily determines the function $A(\mu)$:

$$A(\mu) = -(\eta/36)\, m_b^2 (2q+l) \exp[\tfrac{3}{2}(P/(2q+l))\mu]. \tag{3.20}$$

Now the total change in the Bondi mass can be determined by Eq. (3.5), which in turn requires that $A(\mu = 1) = A(\mu = -1)$, otherwise one would have the situation where the total change of $M(u,\mu)$ would be different in the two opposing directions along the symmetry axis. This then requires that $p = 0$ and therefore $k = 0$. The functions $A(\mu)$ and $B(\mu)$ must then be independent of μ:

$$B(\mu) = m_b, \quad A(\mu) = -(\eta/36)(2q+l)\, m_b^2 \equiv m_a, \tag{3.21}$$

where the constant m_a is introduced so as to simplify the expression for the total mass loss; for which one has simply $\Delta m = -4m_a$. Knowledge of the explicit expressions for A

and B allow one to calculate the integral appearing in Eq. (2.16), and one obtains

$$(\eta/6)(m_b^2 + 2m_a^2) = -6m_a. \tag{3.22}$$

Subtracting this from (3.12) and using (3.14) yields the relationship between q and l:

$$-q = l + 1. \tag{3.23}$$

In order that the constants m_a and m_b be real, it is required that $q < 0$. For ease in interpretation and in order to keep all coefficients real and positive one defines $n = -q$. Therefore, the following equations yield two relationships between the four contants m_a, m_b, η, and n:

$$m_b = \pm \sqrt{2/n}\, m_a, \tag{3.24}$$

$$18n/(n+1) = \eta m_a. \tag{3.25}$$

Equations (3.10) and (3.11) therefore yield explicitly

$$f_3/f_4 = m_a, \tag{3.26}$$

$$(1-\mu^2)^2 f_1^2/f_2 f_4 = m_b^2(1 + n\mu^2)(1-\mu^2). \tag{3.27}$$

From these equations one may now determine expressions for the f_n's. Equation (3.27), with the requirements that f_1 be regular and that the functions f_1 and f_2 be nonzero, imposes the condition that $f_4 = (1-\mu^2)$. Therefore (3.26) requires that $f_3 = m_a(1-\mu^2)$. This finally leaves a certain amount of freedom in the choice of the functions f_1 and f_2 since one has only that

$$f_1^2/f_2 = m_b^2(1 + n\mu^2). \tag{3.28}$$

Thus one arrives at the following expression for $g(u,\mu)$ subject to the relationships (3.24) and (3.25) among the constant parameters:

$$g(u,\mu) = \left[\frac{m_b f(\mu)\, e^{\eta u} + m_a(1-\mu^2)}{f^2(\mu)\, e^{2\eta u} + [1 + (n-1)\mu^2 - n\mu^4]}\right](1 + n\mu^2), \tag{3.29}$$

where $f(\mu)$ is an arbitrary function of μ which must be everywhere regular and positive definite on the interval $-1 \leqslant \mu \leqslant 1$ and $n > 0$. The physical significance of m_a is immediate from (3.5) as it represents one quarter of the total mass loss. When m_a vanishes Eq. (3.24) implies that m_b also vanishes and therefore the function $g(u,\mu)$ is identically zero: the system remains static for all time. The function $g(u,\mu)$ becomes time independent also in the limit $\eta \to 0$ which implies either $m_a \to \infty$ or $n \to 0$. The first situation is not well defined physically since an infinite mass loss would also require an infinite initial mass and the second situation makes the polynomial appearing in (3.11) be of third order in which case one finds that all numerical coefficients vanish and therefore once again $g(u,\mu)$ is identically zero.

IV. PROPERTIES OF THE NEWS FUNCTION AND THE MASS ASPECT

In this section a brief examination of some of the qualitative features associated with the news function and the mass aspect will be made. Considering the arbitrariness of the function $f(\mu)$ appearing in (3.29) and the freedom to choose two parameters, which will undoubtedly be lost once certain conditions are imposed on $N(u,\mu)$ and the higher-order Bondi functions, only certain general properties can be analyzed. In order to be more precise in the discussion to follow, it will be assumed that $f(\mu)$ is an even function of μ and that the condition $f^2(\mu) \geqslant (1 + n\mu^2)(1-\mu^2)$ holds. These requirements do not seem to be overly restrictive since only certain detailed features, which do not affect the general behavior of $g(u,\mu)$ or $M(u,\mu)$ are introduced when these conditions are weakened.

First, depending upon the choice of the sign of m_b, the asymptotic shear $g(u,\mu)(1-\mu^2)$ is seen to undergo two distinctly different forms of evolutionary behavior except of course on the axis where it vanishes identically for all times. Initially, $c(u,\mu)$ will have the value $m_a(1-\mu^2)$ and this is independent of the sign of m_b. However, as the retarded time increases, $c(u,\mu)$ will, in the case where $m_b > 0$ increase to a maximum value and then fall asymptotically to zero as $u \to \infty$. For $m_b < 0$, the evolution is such that the asymptotic shear decreases to a minimum negative value and then increases in order to vanish in the asymptotic future (see Fig. 1). An explicit expression for the news function is obtained by differentiating Eq. (3.29) with respect to the retarded time:

$$\dot{c}(u,\mu) = \frac{\eta f(\mu)\, e^{\eta u}(1-\mu^2)}{[(f^2(\mu)/(1+n\mu^2))\, e^{2\eta u} + (1-\mu^2)]^2} \times \left\{\frac{-m_b f^2(\mu)\, e^{2\eta u}}{1+n\mu^2} - \frac{2m_a(1-\mu^2) f(\mu)\, e^{\eta u}}{1+n\mu^2} + m_b(1-\mu^2)\right\}, \tag{4.1}$$

which outside of vanishing in the asymptotic past and asymptotic future, also vanishes at a finite retarded time determined by the equation

$$\frac{1+n\mu^2}{f(\mu)} e^{-\eta u} - \frac{f(\mu)}{1-\mu^2} e^{\eta u} = \frac{2m_a}{m_b}.$$

Independently of the sign of m_b, the news function reverses its sign once during the entire evolution, and the sign of m_b determines the sign that the news function will have initially. The angular dependence of (4.1) also has the general feature that not only does the amplitude of the news function increase as one moves off of the axis of symmetry, but also

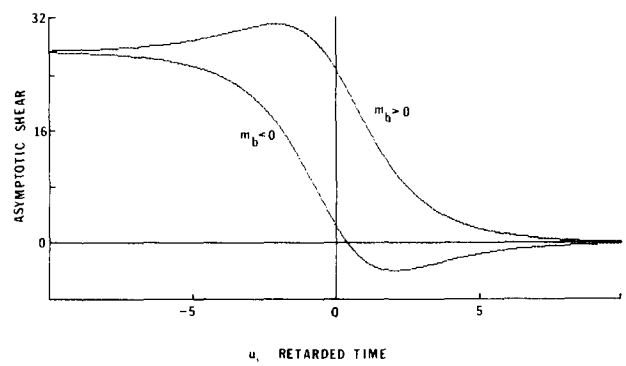

FIG. 1. A plot of the time dependence of the asymptotic shear on the equatorial plane ($\mu = 0$) for $m_a = 27$ and $n = 3$. The evolution undergoes two distinct forms of behavior depending upon the choice for the sign of m_b in Eq. (3.24).

the time at which the news function reverses its sign increases as θ increases from zero to $\pi/2$. This behavior is shown in Fig. 2. For $m_b > 0$ the time at which the sign reversal occurs never exceeds $u = 0$, whereas for $m_b < 0$ this time is also bounded but that bound may be either negative or positive depending upon the value of n.

It is of interest to compare the behavior of the news function (4.1) with certain axisymmetric dynamic space-times involving zero impact parameter collisions particularly the two black hole collision problem considered by D'Eath[9] who analyzed the case where the two bodies approach each other with nearly the velocity of light. Using a perturbation calculation, he was able to obtain an expression for the leading term of the news function at angles close to the forward direction, $\theta = 0$. The behavior of the news function calculated by D'Eath is similar to the behavior of (4.1) for the case $m_b < 0$, i.e., the amplitude before sign reversal is negative and the absolute values of the minimum and maximum increase with an increase in the angle θ (for $\theta \sim 0$).

Two other axisymmetric collision space-times which show similar features are those analyzed by Davis *et al.*[13] who, using perturbation methods, analyzed the radiation from a small particle falling radially into a Schwarzschild black hole and by Smarr[14] who, employing a numerical computation, studied the head-on collision of two equal-mass black holes. Qualitatively the radiative part of the metric which determines the mass loss in the two examples above, demonstrate (modulo the "ringing tails" associated with the normal mode vibrations of the final black hole) the same behavior as the news functions determined by D'Eath and that of Eq. (4.1). Despite these similarities however, the sources and their motions which lead to the news function (4.1) must be considered to be unknown at the present time.

The expression for $g(u, \mu)$ also allows the initial and final values of $F(\mu)$ to be determined. In the asymptotic past and future one has

$$\lim_{u \to -\infty} g(u, \mu) = m_a,$$

which implies

$$F_{-\infty}(\mu) = -m_a \mu^2 + \kappa_1 \mu + \kappa_2,$$

and

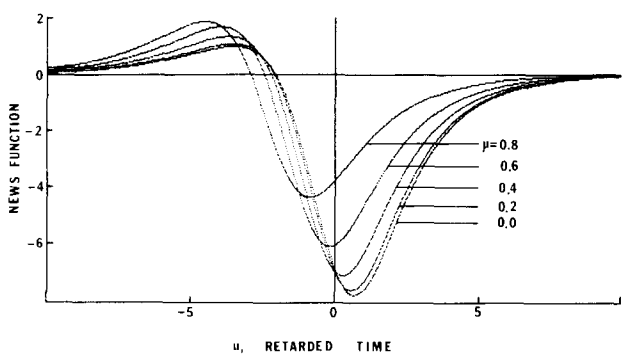

FIG. 2. A plot of the time dependence of the news function for various values of cos θ ($\mu = 1$ on the axis of symmetry). The parameters m_a and n are the same as those for Fig. 1 and m_b is positive.

$$\lim_{u \to \infty} g(u, \mu) = 0,$$

which implies

$$F_{\infty}(\mu) = c_1 \mu + c_2,$$

where c_1, c_2, κ_1, κ_2 are constants. The coordinates system is now determined up to a linear function of μ. While the requirements placed upon the total change of the mass aspect will not impose any new conditions on the functions, $F_{\pm\infty}(\mu)$, one sees that Eqs. (2.13) will determine the constants c_1 and κ_1 if the functions $N(u, \mu)$ and $C(u, \mu)$, etc., are to take on their Weyl expressions at the end of the evolution. All that will be left then as a coordinate freedom would be the liberty to renumber the light cones, $u = \text{const}$, which would have no effect on any of the expressions that determine the total change of the Bondi functions.

A determination of the numerical coefficient associated with the Bondi mass loss would require an explicit knowledge of the function $f(\mu)$, but one can determine the exact behavior of the mass aspect by integrating Eq. (2.11) with respect to retarded time over the interval $-\infty \leqslant \bar{u} \leqslant u$:

$$M(u, \mu) = M(-\infty) - (1-\mu^2)^2 \int_{-\infty}^{u} \dot{g}^2(\bar{u}, \mu)\, d\bar{u} - \tfrac{1}{2}[\, g(u, \mu)(1-\mu^2)^2]'' + 2(3\mu^2 - 1)\, m_a. \tag{4.2}$$

After a rather straightforward but tedious calculation one obtains

$$M(u, \mu) = M(-\infty) - 4m_a + \left(\frac{f^2(\mu)\, e^{2\eta u}}{1 + n\mu^2} + (1-\mu^2)\right)^{-3} \times \left[4m_a(1-\mu^2)^3 + \sum_{l=1}^{5} H_l(\mu)\, e^{l\eta u}\right], \tag{4.3}$$

where the explicit expressions for the functions $H_l(\mu)$ ($l = 1 - 5$) are given in the Appendix. Clearly the simple relationship that exists between the Bondi mass and the mass aspect when the system is static is lost once the system becomes time dependent and the nonlinearities of Einstein's equations are taken into account.

Knowing explicitly the function $g(u, \mu)$ and $M(u, \mu)$ allows one to calculate all terms in the Riemann tensor to order r^{-3}. The mass aspect is then a quantity that can be measured and therefore its behavior with respect to time is important. In the asymptotically distant past the mass aspect is simply given by the value $M(-\infty)$ since the term $-4m_a$ is canceled by the first term appearing in the square brackets as $u \to -\infty$. As $u \to \infty$ the last term in (4.3) vanishes and once again the mass aspect is independent of μ; being smaller than its initial value by the amount $4m_a$. From Eqs. (A1)–(A5) one sees that during much of the evolution the changes in the mass aspect occur at angles predominantly transverse to the symmetry axis. Only at late times in the evolution when the coefficients of $e^{5\eta u}$ begin to exert their greatest effect will there be any significant changes of M on the axis. Choosing $m_b > 0$, the time at which the mass aspect undergoes a collapse on the axis equal to one half the total mass loss is found to be

$$u_c = \frac{1}{2\eta} \ln \frac{8(n+1)^2}{nf^2(\mu = \pm 1)},$$

whereas, the greatest loss of the Bondi mass will occur as a burst, at a time approximately centered about the time at which the news function undergoes a time reversal (since the amplitude of the news function is a maximum just before and just after that time). Adding the assumptions that $n \geqslant 1$ and that the dominant contribution to the mass loss comes from radiation in the equatorial ($\theta = \pi/2$) direction, the time at which this burst of energy loss occurs is of the order

$$u_b = -(1/2\eta)\ln[2nf(\mu = 0)],$$

which clearly precedes the collapse of the mass aspect on the axis. Most of the energy loss then would probably be due to source motions along the axis of symmetry since the radiation field in weak field regions, being of a transverse nature, vanishes on the axis. The rapid and delayed collapse of the mass aspect near the axis while not contributing significantly to the energy flux must come from some unusual relativistic effect.

Finally this section concludes with some remarks concerning the nature of $N(u, \mu)$. Since both M' and $\dot{g}$ vanish initially and finally, Eq. (2.12) shows that $N(u, \mu)$ will be independent of time at the beginning and at the end of its evolution. However in order to determine the exact final angular dependence of N, Eq. (2.12) must be integrated with respect to u. If $C(u, \mu)$ is to be time independent as $u \to \infty$ then N_{final} must take on its Weyl form, i.e.,

$$\Delta N_{\text{total}} = (1-\mu^2)^{1/2}\,[\Delta D_{\text{total}} + M(-\infty)(c_1 - \kappa_1) - 4m_a c_1 + 2m_a M(-\infty)\mu].$$

This requirement will determine further relationships between η, c_1, κ_1, m_a, and $M(-\infty)$ as well as determine, perhaps, the explicit form of $f(\mu)$. Since there exist only a limited number of parameters and one arbitrary function, it is rather doubtful that one can insure that *all* of the higher-order multipole aspects can be put in their Weyl form as $u \to \infty$. One would therefore expect that the final state while not radiative will not be entirely static either, since there will probably exist some multipole aspects that cannot be made time independent.

V. CONCLUSION

The characteristic initial value problem has certain advantages in that it provides a beautiful hierarchy of equations that may be solved step by step once the initial data is provided. Assuming that there exists an expansion in terms of r^{-1} simplifies the field equations and allows one to calculate exact properties of the asymptotic gravitational field without resorting to perturbation methods where certain dimensionless parameters must remain less than unity. The complete evolutionary behavior of the Riemann tensor far from the sources can then be determined even when relativistic effects become dominant.

Despite the relative ease by which one can arrive at some exact knowledge concerning the nature of gravitational radiation, there do exist a number of disadvantages associated with the r^{-1} expansion, notably the inability to link the behavior of the gravitational field with the motions of the sources. From the arguments presented at the end of the previous section it seems that the Bondi formalism by itself is unable to establish the existence of radiative transitions between two exactly stationary states. As a result the problem of source behavior then becomes more enigmatic since the "wave tails" which would present themselves as time-dependent Bondi functions occurring as coefficients of the higher-order r^{-1} terms in the expansions, clearly make a distinction between exactly stationary and more general nonradiative systems. The existence of the tails also brings into question the validity of the $1/r$ expansion since the convergence of such a method may be upset, especially, if one wishes to analyze the field for all times.

Another problem is that linked with the choice of a "good" coordinate system for which a discussion of radiative fields can be presented as simply as possible. This is evident particularly in the supertranslation freedom that is associated with the arbitrariness in the choice of the initial shear of the null cones. If, in the problem discussed in this work, one had set $g = 0$ initially with a particular choice of $F(\mu)$ then a negative shear would have to develop later in the evolution in order to account for the mass loss. This might be somewhat anti-intuitive since one would ordinarily expect that a dynamic, axially symmetric system would in general tend to decrease its deviation from spherical symmetry over the period of time during which it radiates and that if the coordinate system is properly chosen to be as nearly "spherical" as possible, the shear would be able to measure this decrease of the deviation from spherical symmetry. It is rather satisfying that in a coordinate system chosen to match such an evolution, that the parameter which is related to the total mass loss appears in a self-evident manner.

Finally, the program described in this paper was begun with the hope that the Bondi method could avoid the large quantities of tedious algebraic computations which occur in the known perturbation techniques. Unfortunately the expression for $g(u, \mu)$ is complicated enough that the amount of computational work involved in calculating the higher-order Bondi functions grows enormously with increasing orders. Even at the level of calculating explicitly the time dependence of the mass aspect, this fact begins to present itself. However, there is a good deal more information hidden in the higher-order functions. For example, a result not yet obtained would be the relationship between m_a and $M(-\infty)$ which is not determined by a calculation of the mass loss alone. This is due to the fact that information about how the energy of a system is distributed spatially is required in order that one can determine whether or not a system's total energy is positive and how much of it can be lost. Therefore knowledge of the higher-order functions in the expansion is needed. Furthermore carrying the calculation out to include the functions $N(u, \mu)$ and $C(u, \mu)$ would allow one to determine the Newman–Penrose conserved quantities in an explicit manner without resorting to approximation techniques.

ACKNOWLEDGMENTS

Special thanks go to the Laboratoire de Physique Theorique, Institut Henri Poincaré, for its hospitality and to A. Papapetrou and B. Linet for helpful discussions.

This work was partially supported by a NATO–National Sciences and Engineering Research Council of Canada, Postdoctoral Fellowship which the author held when this work was begun.

APPENDIX: CONTRIBUTIONS TO THE MASS ASPECT

In this appendix the explicit angular dependence of the functions $H_l(\mu)$ appearing in the time-dependent mass aspect are given. The calculation makes use of the relationship

$$m_a = (\eta/24)[m_b^2(1+n\mu^2)+2m_a^2(1-\mu^2)](1-\mu^2) + \tfrac{1}{2}m_a(3\mu^2-1),$$

in order to simplify some otherwise lengthy expressions.

One has then, after substituting (3.29) into (4.2),

$$H_1(\mu) = (m_b/2)(1-\mu^2)^3[(1-\mu^2)f'' - 4\mu f' - 2f], \tag{A1}$$

$$H_2(\mu) = m_a \frac{(1-\mu^2)^2}{1+n\mu^2}\left\{-(1-\mu^2)^2\left[ff'' + (f')^2 - \frac{2n\mu ff'}{1+n\mu^2} + \left(\frac{n(n\mu^2-1)}{(1+n\mu^2)^2} - \eta m_a\right)f^2\right] + 4(1-\mu^2)f\left[f' - \frac{n\mu f}{1+n\mu^2}\right] + f(17\mu^2-5)\right\}, \tag{A2}$$

$$H_3(\mu) = m_b \frac{(1-\mu^2)^2}{(1+n\mu^2)}f\left\{-(1-\mu^2)\left[3(f')^2 - \frac{4n\mu ff'}{1+n\mu^2} + \left(\frac{n(n\mu^2-1)}{(1+n\mu^2)^2} - \frac{4}{3}\eta m_a\right)f^2\right] - 3f^2(f+2\mu f')\right\}, \tag{A3}$$

$$H_4(\mu) = m_a \frac{(1-\mu^2)f^2}{(1+n\mu^2)^2}\left\{(1-\mu^2)^2\left[-ff'' + 3(f')^2 - \frac{6n\mu ff'}{1+n\mu^2} + \frac{n(3n\mu^2+1)}{(1+n\mu^2)^2}\right] + (1-\mu^2)f\left[12\mu\left(f' - \frac{n\mu f}{1+n\mu^2}\right) + \frac{\eta m_b^2 f}{m_a}\right] + 3f^2(5\mu^2-1)\right\}, \tag{A4}$$

$$H_5(\mu) = \frac{m_b f^3}{(1+n\mu^2)^2}\left\{(1-\mu^2)^2\left[-\frac{ff''}{2} + (f')^2 - \frac{4n\mu ff'}{1+n\mu^2} + \frac{n(3n\mu^2+1)}{(1+n\mu^2)^2}\right] + 4\mu(1-\mu^2)f\left[f' - \frac{2n\mu f}{1+n\mu^2}\right] + 2(3\mu^2-1)f^2\right\}. \tag{A5}$$

On the axis ($\mu = \pm 1$) the only nonvanishing contribution comes from the last term appearing in $H_5(\mu)$.

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On the local GL(4, R) gauge symmetry of hyperbolic complex metrics

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(Received 10 February 1984; accepted for publication 15 June 1984)

There exists a construction of hyperbolic complex Lorentz frames for any signature η. We prove GL(4, R) to be locally isomorphic to $U(\eta, H)$ by Lie algebra theory. Therefore, the local GL(4, R) gauge symmetry of hyperbolic complex metric g in the nonsymmetric gravitational theory, in fact, is a symmetry of rotations of the hyperbolic complex Lorentz frames.

PACS numbers: 04.50. + h, 02.40.Ky

I. INTRODUCTION

In order to solve the ghost poles problem in the nonsymmetric gravitational theory,[1] Kunstatter, Moffat, and Malzan[2] suggested a theory in which the metric g of the space-time manifold M takes hyperbolic complex values, and this metric should have an internal GL(4, R) gauge symmetry. Concerning this gauge symmetry, the discussion in Ref. 2 is on the basis of the fiber bundle theory,[3] i.e., the theorem concerning the reduction of the structure group of a principal fiber bundle and the existence of a cross section. In Sec. II of this paper, we prove explicitly that GL(4, R) is locally isomorphic to a group of the hyperbolic complex transformations related to any designative signature η. From an element $A \in$ GL(4, R), the hyperbolic complex unitary transformation, which corresponds to A, can specifically be written out. Kunstatter and Yates[4] have given the ordinary complex frames, corresponding to it, in Sec. III we give the hyperbolic complex Lorentz frames. The local GL(4, R) gauge symmetry of g, in fact, is an evident symmetry of g concerning hyperbolic complex unitary transformations. Therefore, it is clear that the status of GL(4, R) in this nonsymmetric gravitational theory, indeed, completely corresponds to the status of the (real) Lorentz group in general relativity or the group U(3,1) in ordinary Einstein's complex metric theory of gravitation.[1,5] Now, the specific physical and geometric significance of this symmetry is very clear.

II. HYPERBOLIC COMPLEX UNITARY TRANSFORMATIONS GROUP AND GL(4, R)

Let $V = (V^\alpha)$ be a vector of the four-dimensional hyperbolic complex linear space T_H, its components $V^\alpha = u^\alpha + \epsilon v^\alpha$, where $\epsilon^2 = 1$, u^α, and v^α are real, $\alpha = 1,2,3,4$. For designative signature η, we define the norm of V by

$$\|V\|^2 = \eta_{\mu\nu} V^\mu \tilde{V}^\nu, \tag{1}$$

where the symbol "$\sim$" is the conjugation operator $\tilde{V}^\alpha = u^\alpha - \epsilon v^\alpha$. A linear transformation f: $T_H \to T_H$ can be denoted by a 4×4 hyperbolic complex matrix $f = (f^\beta_\alpha)$, and f can be decomposed as

$$f = A + \epsilon B, \tag{2}$$

where A and B are 4×4 real matrices. Here f is called a "hyperbolic complex unitary transformation" (related signature η) if $\|f(V)\| = \|V\|$, for any $V \in T_H$. It is easily proved that f is a hyperbolic complex unitary transformation if and only if

$$AA^\# - BB^\# = I, \tag{3}$$

$$AB^\# - BA^\# = 0, \tag{4}$$

where I is the 4×4 unit matrix, $A^\# = \eta A^T \eta^{-1}$, A^T is the transposed matrix of A. Now, f has the inverse transformation

$$f^{-1} = \eta f^\dagger \eta^{-1}, \tag{5}$$

where $f^\dagger = \tilde{f}^T$. Therefore, all f's form a group U(η, H).

We take U(η, H) as a 16-dimensional real manifold, then we can consider its Lie algebra gl(η, H). If a 4×4 matrix $B = a + \epsilon b$ is an element of gl(η, H), then

$$B\eta - \eta B^\dagger = 0. \tag{6}$$

From Eq. (6) we can find all bases of gl(η, H). For arbitrary signature η the following steps of discussion are applicable. But, in gravitational theory what usually interests us is the case $\eta = \mathrm{diag}(1, -1, -1, -1)$. So, we shall only discuss this case as follows.

Let $\mathscr{E}_{\alpha\beta}$ denote a 4×4 real matrix, its μth line, νth column element is $\delta_{\alpha\mu}\delta_{\beta\nu}$, $a_{\alpha\beta} = 2\mathscr{E}_{(\alpha\beta)} = \mathscr{E}_{\alpha\beta} + \mathscr{E}_{\beta\alpha}$, $b_{\alpha\beta} = 2\mathscr{E}_{[\alpha\beta]} = \mathscr{E}_{\alpha\beta} - \mathscr{E}_{\beta\alpha}$. Then we obtain the following 16 bases (A, d, B) of gl(η, H). The first six are just the bases of the Lie algebra of ordinary Lorentz group: $A_{21} = a_{21}$, $A_{31} = a_{31}$, $A_{41} = a_{41}$, $B_{32} = b_{32}$, $B_{42} = b_{42}$, and $B_{43} = b_{43}$. The rest are $d_\alpha = \epsilon\mathscr{E}_{\alpha\alpha}$, $A_{32} = \epsilon a_{32}$, $A_{42} = \epsilon a_{42}$, $A_{43} = \epsilon a_{43}$, $B_{21} = \epsilon b_{21}$, $B_{31} = \epsilon b_{31}$, and $B_{41} = \epsilon b_{41}$. So, the commutation relation among these bases can easily be written out. Now, we consider the relation between gl(4, R) and gl(η, H). Sixteen bases of gl(4, R) are all $\mathscr{E}$'s. We define a linear transformation ρ: gl(4, R) $\to$ gl(η, H) by

$$\begin{aligned} &\rho(\mathscr{E}_{\alpha\beta}) = \tfrac{1}{2}(A_{\alpha\beta} + B_{\alpha\beta}), \quad \text{when } \alpha > \beta, \\ &\rho(\mathscr{E}_{\alpha\beta}) = \tfrac{1}{2}(A_{\beta\alpha} - B_{\beta\alpha}), \quad \text{when } \alpha < \beta, \\ &\rho(\mathscr{E}_{\alpha\alpha}) = d\alpha. \end{aligned} \tag{7}$$

We can directly examine that ρ is an isomorphic mapping from gl(4, R) to gl(η, H). Therefore, according to the Lie group theory, GL(4, R) is isomorphic to U(η, H) as two local linear Lie groups. For other signatures the above discussion can also be carried out similarly. Thus, the signature η, in fact, is arbitrary, i.e., every U(η, H), which corresponds to some signature η, is locally isomorphic to GL(4, R).

In GL(4, R) an element of the connected component, which contains the unit element, can be written as

$$A = \exp(a)\exp(b)\cdots, \quad a, b, \ldots \in \mathrm{gl}(4, R). \tag{8}$$

Corresponding to A the hyperbolic complex unitary transformation is

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$$f = \exp(\rho(a))\exp(\rho(b))\cdots. \tag{9}$$

Therefore, the effect of GL(4, R) gauge transformation of an element, in fact, can be explained as the effect of a hyperbolic complex unitary transformation.

III. HYPERBOLIC COMPLEX LORENTZ FRAMES

We take GL(4, R) as the local transformation group acting on M. Equations (8) and (9) mean that there is a hyperbolic complex Lorentz frames bundle $L_H(M)$ (related to some η). If $V = \{V_a\} \in L_H(M)$, $a = 1,2,3,4$, and we let the matrix (V^a_μ) be the inverse matrix of $(\tilde{V}^\mu_a)$, then

$$V^a_\mu \tilde{V}^\nu_a = \delta^\nu_\mu, \quad V^b_\mu \tilde{V}^\mu_a = \delta^b_a. \tag{10}$$

If $V(x)$ is a cross section of $L_H(M)$, and a metric g is defined by

$$g_{\mu\nu} = \eta_{ab} V^a_\mu \tilde{V}^b_\nu, \tag{11}$$

then g obviously is invariable under a local hyperbolic complex unitary gauge transformation of V. Conversely, if a local GL(4, R) gauge symmetric metric g exists, then we can prove that there is a $V(x) \in L_H(M)$ and Eq. (11) holds. In fact, according to Ref. 2, there exists now a real metric g'. For the tangent space T_x at each point $x \in M$ we have

$$g'(A', B') = -g'(EA', B'), \quad \forall A, B \in T'_x = T_x \times T_x, \tag{12}$$

$$g(A, B) = g'(A', B') + \epsilon g'(EA', B'), \tag{13}$$

$$E = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix},$$

where $A = (A'^\alpha + \epsilon A'^{\overline{\alpha}})e_\alpha$ and real $\{e_\alpha\}$ spans T_x, $\overline{\alpha} = \alpha + 4$. Equation (12) means that g' corresponds to the signature $H = (\eta, -\eta)$. Now, on M there is an ordinary real Lorentz frame $\{V_A\}$ $(A = 1,2,...,8)$,

$$V'^A_\Gamma V'^\Delta_A = \delta^\Delta_\Gamma, \quad V'^B_\Gamma V'^\Gamma_A = \delta^B_A \quad (\Gamma, \Delta = 1,2,...,8),$$

and

$$g'_{\Gamma\Delta} = H_{AB} V'^A_\Gamma V'^B_\Delta = H_{ab}(V'^a_\Gamma V'^b_\Delta + V'^{\bar{a}}_\Gamma V'^{\bar{b}}_\Delta). \tag{14}$$

Let $V_a = (V'^\alpha_a + \epsilon V'^{\overline{\alpha}}_{\bar{a}})e_\alpha$, then we can directly see that Eq. (10) holds for $H = (\eta, -\eta)$, and

$$\begin{aligned} g_{\mu\nu} &= g(V_\mu, V_\nu) = g'(V'_\mu, V'_\nu) + \epsilon g'(EV'_\mu, V'_\nu) \\ &= H_{AB} V'^A_\mu V'^B_\nu + \epsilon(H_{ab} V'^{\bar{a}}_\mu V'^b_\nu + H_{\bar{a}\bar{b}} V'^a_\mu V'^{\bar{b}}_\nu) \\ &= \eta_{ab} V^a_\mu \tilde{V}^b_\nu. \end{aligned} \tag{15}$$

IV. CONCLUSIONS AND DISCUSSIONS

GL(4, R) is locally isomorphic to a hyperbolic complex unitary group related to any signature η. The GL(4, R) gauge symmetry of the nonsymmetric metric g can be explained as the symmetry of g related to the hyperbolic complex unitary group. There are hyperbolic complex Lorentz frames, the relation between g and these frames is just a direct extension of the relation between a Riemann metric and the ordinary Lorentz frames.

If $\epsilon = 0$, we, of course, obtain the theory of Riemann metric and Lorentz frames.

If $\epsilon^2 = -1$, then g changes into an ordinary Einstein complex metric. When $\eta = \text{diag}(1, -1, -1, -1)$, the local gauge group is U(3,1). Although we can also write out the transformation ρ, now ρ is not an isomorphic mapping of two Lie algebras, i.e., U(3,1) and GL(4, R) are not locally isomorphic. This makes an essential distinction between an ordinary complex metric theory of gravitation and the hyperbolic complex theory of gravitation.

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A generating function for Chew–Mandelstam functions

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(Received 12 January 1982; accepted for publication 25 April 1984)

We have obtained the generating function for Chew–Mandelstam functions for arbitrary integral angular momentum. From this a closed formula for the Chew–Mandelstam functions is derived in both the simple equal mass case and in the more complicated case of unequal masses.

PACS numbers: 11.80.Cr, 11.20.Fm, 11.80.Gw

I. INTRODUCTION

There exists a variety of approximate representations of the S matrix. In this paper we look at the K matrix approximation for the multichannel scattering matrix $\mathscr{S}_l(s)$ in the lth partial wave[1–4]:

$$\mathscr{S}_l = 1 + 2i\rho_l^{1/2} T_l \rho_l^{1/2}, \tag{1.1}$$

where

$$T_l = K(s)(1 - C_l(s)K(s))^{-1} \tag{1.2}$$

and

$$\rho_l = \operatorname{Im} C_l \tag{1.3}$$

is a diagonal matrix of two-body phase-space factors. $K(s)$ is a real, symmetric matrix whose elements are meromorphic functions of s, the invariant squared energy. At threshold

$$\rho_l \propto (2k/\sqrt{s}) \cdot k^{2l}, \tag{1.4}$$

where k is the center-of-mass three-momentum, $k^2 = (s-a)(s-b)/4s$ and the convenient abbreviations $a = (m_1 + m_2)^2$, $b = (m_1 - m_2)^2$ have been introduced. The functions C_l will be assumed to satisfy the dispersion relation

$$\operatorname{Re} C_l(s) = \frac{s}{\pi} \int_a^\infty ds' \frac{\operatorname{Im} C_l(s')}{s'(s'-s)}. \tag{1.5}$$

We wish to focus on the Chew–Mandelstam functions singled out for extensive application for Edwards and Thomas.[3] These they define by setting

$$\rho_l = \left(\frac{2k}{\sqrt{s}}\right)\left(\frac{2k}{\sqrt{s}}\right)^{2l} \theta(s-a), \tag{1.6}$$

which satisfies both the threshold requirement Eq. (1.4) and allows the C_l to obey the once-subtracted dispersion relation Eq. (1.5) via Eq. (1.3). This choice of ρ_l is more general than it first appears, incorporating the correct threshold behavior and also allowing for approximations to be made to the left-hand singularities by choice of the meromorphic elements of the K matrix.

Assume, contrary to Eq. (1.6), that

$$\rho_l = \operatorname{Im} \tilde{C}_l = (2k/\sqrt{s})(2k/b)^{2l}, \tag{1.7}$$

where b is a real constant. ρ_l satisfies the threshold requirements. $\tilde{C}_l(s)$ obeys an $l+1$th subtracted dispersion relation

$$\tilde{C}_l(s) = \sum_{n=0}^{l} \frac{\tilde{C}_l^n(0)s^n}{n!} + \frac{s^{l+1}}{\pi} \int \frac{ds'(2k'/\sqrt{s'})(2k'/b)^{2l}}{s'^{l+1}(s'-s-i\epsilon)}, \tag{1.8}$$

where the $l+1$ subtraction constants $\tilde{C}_l^n(0)$ are the nth derivatives of $\tilde{C}_l(s)$ at $s=0$.

This may be written in the more revealing form

$$\tilde{C}_l(s) = P_l(s) + (s^l/b^{2l})C_l(s) \tag{1.9}$$

and

$$C_l(s) = \frac{s}{\pi} \int \frac{ds'(2k'/\sqrt{s'})^{2l+1}}{s'(s'-s-i\epsilon)}. \tag{1.10}$$

$P_l(s)$ is an lth degree polynomial in s, and $C_l(s)$ are precisely the Chew–Mandelstam functions as defined by Eq. (1.6).

The unknown polynomial coefficients may be absorbed into the K matrix elements so that the S matrix may be written in K matrix form either with the functions as here defined by Eq. (1.7) or in terms of the Chew–Mandelstam functions as Edwards and Thomas do. We conclude that the Chew–Mandelstam functions may appear even if the ansatz Eq. (1.6) is not imposed.

By contrast both Cutkosky *et al.*[5] and Törnqvist[6] use model-dependent modifications of ρ_l: in the first case to simulate left-hand cut structure with parameter-dependent terms in ρ_l, in the latter case by the addition of parameter-dependent damping factors to enable the modified C_l to satisfy a once-subtracted dispersion relation.

Although Edwards and Thomas gave explicit forms for the C_l for small l, no general expression was written down. In this paper we exhibit a useful closed form for these functions. We proceed in two stages. First, we find the generating function $C(s,z)$ for the functions $C_l(s)$. This is defined by the formal power series expansion in z

$$C(s,z) = \sum_{l=0}^{\infty} C_l(s) z^l. \tag{1.11}$$

Having found $C(s,z)$, we use it to obtain a closed form for the $C_l(s)$.

II. THE GENERATING FUNCTION

From Eqs. (1.5) and (1.7) we see that $C(s,z)$ satisfies the same once subtracted dispersion relation as the $C_l(s)$, namely

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$$\mathrm{Re}\, C(s,z) = \frac{s}{\pi}\int_a^\infty ds' \frac{\mathrm{Im}\, C(s',z)}{s'(s'-s)}. \tag{2.1}$$

Further,

$$\mathrm{Im}\, C(s,z) = \sum_{l=0}^{\infty}\left(\frac{2k}{s^{1/2}}\right)^{2l+1} z^l = \frac{2k}{s^{1/2}}\left(1-\frac{4k^2 z}{s}\right)^{-1}. \tag{2.2}$$

Hence

$$C(s,z) = \frac{s}{\pi}\int_a^\infty ds' \frac{(s'-a)(s'-b)}{(s'-s-i\epsilon)} \frac{1}{(s'-a)^{1/2}(s'-b)^{1/2}P(s')}, \tag{2.3}$$

where

$$P(s) = (1-z)s^2 + z(a+b)s - zab. \tag{2.4}$$

At this point we remark that

$$\frac{(s'-a)(s'-b)}{(s'-s)} = s' + (s-a-b) + \frac{(s-a)(s-b)}{(s'-s)}. \tag{2.5}$$

It has proven most convenient to split the integration in Eq. (2.3) into three parts in the fashion suggested by Eq. (2.5). Then the integrations can all be done in terms of elementary functions[7] (for details see Appendix A) and we obtain

$$C(s,z) = I_1 + I_2 + I_3, \tag{2.6}$$

$$C_l(s) = I_{1,l} + I_{2,l} + I_{3,l}, \tag{2.7}$$

$$I_1 = \frac{2k}{\pi s^{1/2}}\left(1-\frac{4k^2 z}{s}\right)^{-1} \times\left[-2\ln\left(\frac{(s-a)^{1/2}+(s-b)^{1/2}}{2(m_1 m_2)^{1/2}}\right)+i\pi\right], \tag{2.8}$$

$$I_2 = \frac{1}{\pi}\left(1-\frac{4k^2 z}{s}\right)^{-1}\frac{1}{2z^{1/2}}\ln\left|\frac{1+z^{1/2}}{1-z^{1/2}}\right|, \tag{2.9}$$

$$I_3 = \frac{1}{\pi}\left(1-\frac{4k^2 z}{s}\right)^{-1}\left(\frac{a+b}{2}-\frac{ab}{s}\right)\frac{Q}{(a+b)}\ln\left|\frac{1+Q}{1-Q}\right|, \tag{2.10}$$

where

$$Q = \frac{(a+b)}{2}\left(ab + \frac{z(a-b)^2}{4}\right)^{-1/2}. \tag{2.11}$$

Note that $C(s,0)$ correctly reproduces the expression for the S wave Chew–Mandelstam function $C_0(s)$ given in Basdevant and Berger. In general one has from Eq. (1.7)

$$C_l(s) = \frac{1}{l!}\frac{d^l C(s,z)}{dz^l}, \quad z=0. \tag{2.12}$$

However, it is not necessarily trivial to find from Eqs. (2.8)–(2.12) the explicit expressions for $C_l(s)$. The three parts I_1, I_2, I_3 differ very considerably in the ease with which they yield up the closed expressions. For example, we can write almost immediately

$$I_{1,l} = -\frac{2}{\pi}\left(\frac{2k}{s^{1/2}}\right)^{2l+1}\ln\left(\frac{(s-a)^{1/2}+(s-b)^{1/2}}{2(m_1 m_2)^{1/2}}\right) + i\left(\frac{2k}{s^{1/2}}\right)^{2l+1}. \tag{2.13}$$

On the other hand I_2 and I_3 require more discussion which we defer to the next section. We give separate treatment for the equal and unequal mass cases.

III. THE CLOSED EXPRESSIONS

A. The equal mass case: $m_1 = m_2 = m$

In this case matters simplify remarkably because Q reduces to $z^{-1/2}$, whence $I_2 = I_3$ and

$$C(s,z) = I_1 + 2I_2, \tag{3.1}$$

$$C(s,z) = \frac{2k}{\pi s^{1/2}}\left(1-\frac{4k^2 z}{s}\right)^{-1} \times\left[-2\ln\left(\frac{(s-4m^2)^{1/2}+s^{1/2}}{2m}\right)+i\pi\right] + \frac{2}{\pi}\left(1-\frac{4k^2 z}{s}\right)^{-1}\frac{1}{2z^{1/2}}\ln\left|\frac{1+z^{1/2}}{1-z^{1/2}}\right|. \tag{3.2}$$

To simplify notation now and later let us introduce the abbreviations:

$$\lambda = \frac{4k^2}{s};\quad \mu = \frac{(a-b)^2}{16ab};\quad \nu = \frac{a+b}{2(ab)^{1/2}};\quad \omega = \nu - \frac{(ab)^{1/2}}{s}. \tag{3.3}$$

Now

$$\frac{1}{2z^{1/2}}\ln\left|\frac{1+z^{1/2}}{1-z^{1/2}}\right| = \sum_{r=0}^{\infty}\frac{z^r}{2r+1}. \tag{3.4}$$

If Eq. (3.4) is multiplied by $(1-\lambda z)^{-1}$ and the result expanded in powers of z, one finds

$$2I_{2,l} = \frac{2}{\pi}\sum_{r=0}^{l}\frac{\lambda^{l-r}}{2r+1}. \tag{3.5}$$

Recalling Eq. (2.13), we finally get

$$\mathrm{Im}\, C_l(s) = \lambda^{l+1/2}, \tag{3.6}$$

$$\mathrm{Re}\, C_l(s) = \frac{2}{\pi}\left[-\lambda^{l+1/2}\ln\left(\frac{(s-4m^2)^{1/2}+s^{1/2}}{2m}\right) + \sum_{r=0}^{l}\frac{\lambda^{l-r}}{2r+1}\right]. \tag{3.7}$$

B. The general case: $m_1 \neq m_2$

In this case we can still use Eqs. (2.13) and (3.5) to find $I_{1,l}$ and $I_{2,l}$, but further work is required to obtain $I_{3,l}$. I_3 can be written as follows:

$$I_3 = \frac{(ab)^{1/2}\omega}{2\pi} WXY, \tag{3.8}$$

where

$$W = (1-\lambda z)^{-1}, \tag{3.9}$$

$$X = 2Q/(a+b), \tag{3.10}$$

$$Y = \ln|(1+Q)/(1-Q)|, \tag{3.11}$$

and $Q(z)$ is given by Eq. (2.11). Then the nth derivatives of W, X, Y with respect to z at $z=0$ are

$$\frac{d^n W}{dz^n} = n!\lambda^n;\quad \frac{d^n X}{dz^n} = \frac{(-1)^n 2^n (2n-1)!!\mu^n}{(ab)^{1/2}};$$

$$Y = 2\ln\left(\frac{m_1}{m_2}\right);$$

$$\frac{d^n Y}{dz^n} = \nu(n-1)! \sum_{p=0}^{n-1} \frac{(-1)^p 2^p (2p-1)!! \mu^p}{p!},$$

for $n > 0$. (3.12)

At this point we introduce a further abbreviation:

$$\Omega(n) = (-1)^n 2^n (2n-1)!!/n!. \tag{3.13}$$

For the detailed proof of Eq. (3.12) see Appendix B. We now take the l th derivative of I_3 and using Eq. (3.12) in conjunction with Leibnitz's rule find at last the following closed expression for $C_l(s)$ in the general case:

$$\text{Im } C_l(s) = \lambda^{l+1/2} \tag{3.14}$$

$$\text{Re } C_l(s) = \frac{1}{\pi}\left[-2\lambda^{l+1/2} \ln\left(\frac{(s-a)^{1/2} + (s-b)^{1/2}}{2(m_1 m_2)^{1/2}}\right) + \sum_{n=0}^{l} \frac{\lambda^{l-n}}{2n+1}\right] + \frac{\omega}{\pi} \ln\left(\frac{m_1}{m_2}\right) \sum_{n=0}^{l} \Omega(n) \lambda^{l-n} \mu^n + \frac{\omega\nu}{2\pi} \sum_{p=1}^{l} \frac{1}{p} \left(\sum_{q=0}^{l-p} \Omega(q) \lambda^{l-q-p} \mu^q\right)\left(\sum_{r=0}^{p-1} \Omega(r) \mu^r\right). \tag{3.15}$$

IV. CONCLUSION

We have found the generating function $C(s, z)$ for the Chew–Mandelstam functions $C_l(s)$ used by Edwards and Thomas. From $C(s, z)$ we have derived a closed form for the $C_l(s)$ in the general case of unequal masses. The advantages of proceeding in this seemingly indirect fashion are well known to mathematicians. As well as being elegant and giving greater power in dealing with refractory expressions, this method may afford insights denied to a more piecemeal approach. One example of this here is the discussion of the equal mass limit. At the level of the generating function [see Eqs. (2.8)–(2.10)] it is trivial to take the equal mass limit $a \to 4m^2$, $b \to 0$. But to do this at the level of the Chew–Mandelstam functions themselves requires a painstaking discussion of the cancellations between divergent terms [see Eq. (3.15)].

ACKNOWLEDGMENTS

The first-named author acknowledges the support of the University of Nairobi, Kenya, where this work was done.

APPENDIX A: THE INTEGRATIONS

$$\text{Re } C(s, z) = \frac{s}{\pi} \int_a^\infty ds' J(s'), \tag{A1}$$

where

$$J(s') = \frac{(s'-a)(s'-b)}{(s'-s) P(s') R(s')^{1/2}}, \tag{A2}$$

and

$$R(s) = (s-a)(s-b), \tag{A3}$$

$$P(s) = (1-z)s^2 + z(a+b)s - zab = s^2 - z(s-a)(s-b) = s(s - 4k^2 z). \tag{A4}$$

Now use

$$\frac{(s'-a)(s'-b)}{(s'-s)} = s' + (s-a-b) + \frac{(s-a)(s-b)}{(s'-s)} \tag{A5}$$

to write

$$J(s') = J_1 + J_2 = \frac{E}{(s'-s) R(s')^{1/2}} + \frac{F + Gs'}{P(s') R(s')^{1/2}}, \tag{A6}$$

where

$$E = \frac{(s-a)(s-b)}{P(s)}, \tag{A7}$$

$$F = s - a - b - \frac{(s-a)(s-b)}{s}\left(\frac{zab}{P(s)} + 1\right), \tag{A8}$$

$$G = 1 - \frac{(s-a)(s-b)(1-z)}{P(s)}. \tag{A9}$$

Let

$$I_1 = \frac{s}{\pi} \int_a^\infty ds' J_1(s'). \tag{A10}$$

Make the substitution $t = (s'-s)^{-1}$ and use Eq. (2.261) on page 81 of Ref. 7 to get

$$I_1 = \frac{2k}{\pi s^{1/2}}\left(1 - \frac{4k^2 z}{s}\right)^{-1} \times \left[-2 \ln\left(\frac{(s-a)^{1/2} + (s-b)^{1/2}}{2(m_1 m_2)^{1/2}}\right) + i\pi\right]. \tag{A11}$$

Hence Eq. (2.8) is proved.

Now look at

$$L = \frac{s}{\pi} \int_a^\infty ds' J_2(s'). \tag{A12}$$

Make the substitution

$$s' = \beta t (1+t)^{-1},$$

where

$$\beta = 2ab/(a+b). \tag{A13}$$

Then L can be brought to the form

$$L = \frac{s\beta}{\pi(1-z)} \int_{a/(\beta-a)}^{-1} dt \frac{A + Bt}{(t^2+x)(t^2+y)^{1/2}}, \tag{A14}$$

where

$$A = -i\frac{(a+b)^3 (ab)^{-3/2}}{(a-b)} [4ab + z(a-b)^2]^{-1} F, \tag{A15}$$

$$B = GA/F, \tag{A16}$$

$$x = -z(a+b)^2/[(a-b)^2 z + 4ab], \tag{A17}$$

$$y = -(a+b)^2/(a-b)^2. \tag{A18}$$

Break L into two parts:

$$L = I_2 + I_3, \tag{A19}$$

$$I_2 = \frac{s\beta}{\pi(1-z)} \int_{a/(\beta-a)}^{-1} dt \frac{A}{(t^2+x)(t^2+y)^{1/2}}, \tag{A20}$$

$$I_3 = \frac{s\beta}{\pi(1-z)} \int_{a/(\beta-a)}^{-1} dt \frac{Bt}{(t^2+x)(t^2+y)^{1/2}}. \tag{A21}$$

In I_2 make the substitution $t^2 = -v^2(t^2+y)$ as suggested in Sec. 2.25 of Ref. 7. After some elementary steps, one finally gets

$$I_2 = \frac{1}{\pi}\left[1 - \frac{4k^2 z}{s}\right]^{-1} \frac{1}{2z^{1/2}} \ln\left|\frac{1+z^{1/2}}{1-z^{1/2}}\right| \tag{A22}$$

and Eq. (2.9) is proved. In I_3 make the substitution $t^2 + y = -u^2$. Again after some work, one finds

$$I_3 = \frac{1}{\pi}\left[1 - \frac{4k^2 z}{s}\right]^{-1}\left[\frac{a+b}{2} - \frac{ab}{s}\right]\frac{Q}{(a+b)} \ln\left|\frac{1+Q}{1-Q}\right|, \tag{A23}$$

where

$$Q = \frac{(a+b)}{2}\left[ab + \frac{z(a-b)^2}{4}\right]^{-1/2} \tag{A24}$$

and Eq. (2.10) is proved.

One might worry that $C(s, z)$ could have singularities in the z-plane which would invalidate the expansion around $z = 0$ in Eq. (1.7). Fortunately this is not so. Look at Eqs. (2.8)–(2.10). I_1, I_2, I_3 all have the simple pole at

$$z = \frac{s}{4k^2} = \frac{(1-a)^{-1}}{s}\frac{(1-b)^{-1}}{s}.$$

But $s \geqslant a > b$, hence the pole is always at $z \geqslant 1$. I_1 has no other singularities in z. I_2, I_3 both have a branch point at $z = 1$. Despite appearances, I_2 does not have a branch point at $z = 0$, nor does I_3 have one at

$$z = -\frac{4ab}{(a-b)^2} = -\frac{(m_1^2 - m_2^2)^2}{4m_1^2 m_2^2}.$$

These are the only singularities for finite z. Therefore the expansion (1.7) is valid.

APPENDIX B: THE RECURSION RELATIONS

Given

$$W = (1 - \lambda z)^{-1}, \tag{B1}$$

$$X = 2Q(a+b)^{-1}, \tag{B2}$$

$$Y = \ln|(1+Q)/(1-Q)|, \tag{B3}$$

with

$$Q = \frac{(a+b)}{2}\left[ab + \frac{z(a-b)^2}{4}\right]^{1/2} \tag{B4}$$

and

$$\Omega(n) = (-1)^n 2^n (2n-1)!!/n! \tag{B5}$$

one must show that

$$\frac{1}{n!}\frac{d^n W}{dz^n} = \lambda^n, \tag{B6}$$

$$\frac{1}{n!}\frac{d^n X}{dz^n} = \frac{\Omega(n)\mu^n}{(ab)^{1/2}}, \tag{B7}$$

$$\frac{1}{n!}\frac{d^n Y}{dz^n} = \frac{\nu}{n}\sum_{p=0}^{n-1} \Omega(p)\mu^p \quad \text{for } n > 0, \tag{B8}$$

$$Y = 2\ln\left[\frac{m_1}{m_2}\right]; \quad \text{all at } z = 0. \tag{B9}$$

(B6) is trivial and follows at once from (B1). From (B2) one has

$$X = 2Q(a+b)^{-1} = (ab)^{-1/2}[1 + 4\mu z]^{-1/2} \tag{B10}$$

[recall the abbreviations μ, λ, ν from Eq. (3.3)].

Expanding (B10) in powers of z yields

$$X = (ab)^{-1/2}\sum_{n=0}^{\infty} 4^n z^n \mu^n \binom{-\frac{1}{2}}{n}, \tag{B11}$$

where $\binom{n}{r}$ is the binomial coefficient. The coefficient of z^n is

$$\frac{(-1)^n 4^n \mu^n (2n-1)!!(ab)^{-1/2}}{2^n n!} = \frac{\Omega(n)\mu^n}{(ab)^{1/2}}$$

and so (B7) is proved. Introduce the useful abbreviations

$$\alpha = 4\mu; \quad \beta = \frac{a+b}{2}; \quad \gamma = ab; \quad \delta = \frac{(a-b)^2}{4};$$

$$\nu = \frac{a+b}{2(ab)^{1/2}}; \quad Y^n = \frac{d^n Y}{dz^n}. \tag{B12}$$

Then from (B3)

$$Y^0 = \ln\left[\frac{\beta + (\gamma + \delta z)^{1/2}}{\beta - (\gamma + \delta z)^{1/2}}\right]. \tag{B13}$$

Further it will be shown that for $n > 0$,

$$Y^n = \frac{\nu S_n(z)}{2^{n-1}(1-z)^n(1+\alpha z)^{n-1/2}}, \tag{B14}$$

where $S_n(z)$ satisfies the recursion rule

$$S_{n+1}(z) = \frac{2\,dS_n(z)}{dz}[1 + (\alpha - 1)z - \alpha z^2] + S_n(z)[2n(1-\alpha) + \alpha + \alpha z(4n-1)]] \tag{B15}$$

with the initial conditions

$$S_1 = 1, \quad \frac{dS_1}{dz} = 0. \tag{B16}$$

Take the logarithmic derivative of Eq. (B14) to find

$$\frac{d}{dz}(\ln Y^n) = \frac{1}{S_n}\frac{dS_n}{dz} + \frac{n}{1-z} + \frac{\alpha(\frac{1}{2} - n)}{1+\alpha z}. \tag{B17}$$

Multiply (B17) by Y^n to get

$$Y^{n+1} = \frac{\nu[2(1-z)(1+\alpha z)(dS_n/dz) + 2S_n[n(1+\alpha z) + \alpha(\frac{1}{2} - n)(1-z)]]}{2^n(1-z)^{n+1}(1+\alpha z)^{n+1/2}}. \tag{B18}$$

Comparison of (B14) and (B18) then proves (B15) by induction from Y^1. In particular, (B16) is easily established by differentiating (B13) once. Introduce the notation for the coefficients of the polynomial

$$S_n(z) = \sum_{i=0}^{n-1} S_n^i z^i. \tag{B19}$$

Then Eq. (B15) translates into the following recursion rule for the S_n^i:

$$S^k_{n+1} = 2(k+1)S^{k+1}_n + [2(n-k) - \alpha(2(n-k)-1)] \times S^k_n + \alpha[2(2n-k)+1]S^{k-1}_n, \tag{B20}$$

where S^q_b is always zero for $a \geqslant b$. The solution to (B20) which satisfies the initial conditions (B16) is

$$S^k_n = \binom{n-1}{n-k-1} \frac{(2n-1)!!\alpha^k 2^{n-k-1}(n-k-1)!}{(2n-2k-1)!!} \times \sum_{p=0}^{n-k-1} \frac{(-1)^p(2p-1)!!\alpha^p}{2^p p!}. \tag{B21}$$

Here $\binom{n}{r}$ denotes the binomial coefficient and the double factorial notation is explained in Sec. III. Equation (B21) can then be established from (B20) by induction on n. This lengthy algebra will not be reproduced here. From (B19) and (B21) one has

$$S_n(0) = S^0_n = 2^{n-1}(n-1)! \sum_{p=0}^{n-1} \frac{\Omega(p)\alpha^p}{4^p}. \tag{B22}$$

Combining this result with (B14) one finds

$$\frac{1}{n!} Y^n(z=0) = \frac{\nu}{n} \sum_{p=0}^{n-1} \Omega(p)\mu^p \quad \text{for } n>0,$$

proving Eq. (B8). Equation (B9) follows at one from putting $z=0$ in (B3). Thus finally Eq. (B6) to (B9) are proved.

To establish (3.15), recall (3.8):

$$I_3 = \frac{(ab)^{1/2}\omega WXY}{2\pi}. \tag{B23}$$

By Leibniz's rule one has

$$\frac{d^l I_3}{dz^l} = \frac{(ab)^{1/2}\omega}{2\pi} \sum_{p=0}^{l} \binom{l}{p} Y^p \sum_{q=0}^{l-p} \binom{l-p}{q} W^{l-p-q} X^q, \tag{B24}$$

where the obvious notation $Y^n = \dfrac{d^n Y}{dz^n}$, $Y^0 = 0$, etc. has been used. Hence,

$$\frac{d^l I_3}{dz^l} = \frac{(ab)^{1/2}\omega}{2\pi} \left[\binom{l}{0} Y \sum_{q=0}^{l} \binom{l}{q} W^{l-q} X^q + \sum_{p=1}^{l} \binom{l}{p} Y^p \sum_{q=0}^{l-p} \binom{l-p}{q} W^{l-p-q} X^q \right] \tag{B25}$$

and

$$\frac{d^l I_3}{dz^l} = \frac{(ab)^{1/2}\omega}{2\pi} \left[2\ln\left(\frac{m_1}{m_2}\right) \sum_{q=0}^{l} \binom{l}{q} \frac{(l-q)!\lambda^{l-q} q! \Omega(q)\mu^q}{(ab)^{1/2}} + \sum_{p=1}^{l} \binom{l}{p} \frac{p!\nu^p}{p} \sum_{r=0}^{p-1} \Omega(r)\mu^r \sum_{q=0}^{l-p} \binom{l-p}{q} \times \frac{(l-p-q)!\lambda^{l-p-q} q! \Omega(q)\mu^q}{(ab)^{1/2}} \right]. \tag{B26}$$

So

$$\frac{1}{l!} \frac{d^l I_3}{dz^l} = \frac{\omega}{\pi} \ln\left(\frac{m_1}{m_2}\right) \sum_{n=0}^{l} \Omega(n)\lambda^{l-n}\mu^n + \frac{\omega\nu}{2\pi} \sum_{p=1}^{l} \frac{1}{p} \left[\sum_{q=0}^{l-p} \Omega(q)\lambda^{l-p-q}\mu^q \right] \left[\sum_{r=0}^{p-1} \Omega(r)\mu^r \right]. \tag{B27}$$

Combining this result with those for $I_{1,l}$ and $I_{2,l}$ one gets at long last Eq. (3.15).

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An Sp(3,R)×O($N-1$) basis for the nuclear shell model

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(Received 19 August 1983; accepted for publication 22 June 1984)

An Sp(3,R)×O($N-1$) basis of wave functions is constructed for the nuclear shell model. Such a basis is important because Sp(3,R) is the dynamical group and O($N-1$) the symmetry group for a unified independent particle-collective model of the nucleus. It is needed for the diagonalization of a microscopic shell model Hamiltonian and the interpretation of the collective content of its eigenstates.

PACS numbers: 21.60.Ev, 02.20.Qs, 02.20.Rt, 03.65.Fd

I. INTRODUCTION

The independent particle and collective models of the nucleus have recently been unified in the algebraic Sp(3,R) model.[1] The dynamical group Sp(3,R) of this model not only contains the harmonic-oscillator shell model Hamiltonian in its Lie algebra, it also contains SU(3), the symmetry group of the harmonic oscillator, and CM(3), the dynamical group for collective motion in three dimensions, as subgroups. Sp(3,R) is itself a subgroup of the full dynamical group Sp(3N,R) for the N-particle harmonic oscillator in three dimensions. Thus the Sp(3,R) model is a submodel of the full interacting shell model.

The Sp(3,R) model is a unified model in the sense that both independent particle and collective Hamiltonians are contained in its enveloping algebra. Thus the eigenfunctions of a unified model Hamiltonian lie within the Sp(3,R) irreducible representation spaces. It is therefore of considerable interest to perform fully microscopic shell model calculations in an Sp(3,R) basis[2] to see if collective states emerge and to discover the goodness of Sp(3,R) symmetry. As a prelude to such calculations, we consider the construction of an explicit Sp(3,R) basis of shell model wave functions.

An intrinsic dynamical group, that is complementary to Sp(3,R), is O($N-1$), the group of orthogonal transformations of the N- nucleon coordinates after removal of the center-of-mass.[3] Since the O($N-1$) and Sp(3,R) actions commute, nuclear shell model states can be classified according to their transformation properties under both groups. In this paper, we show how to construct a shell model basis that reduces the subgroup chains

$$\begin{aligned} &\mathrm{Sp}(3,R)\supset \mathrm{U}(3)\supset \mathrm{SU}(3)\supset \mathrm{SO}(3),\\ &\mathrm{O}(N-1)\supset S_N, \end{aligned} \tag{1}$$

where U(3) is the symmetry group of the harmonic-oscillator Hamiltonian and S_N is the symmetric group of space permutations.[4] The presence of S_N is important because it means that spin-isospin wave functions of symmetry contragredient to that of the Sp(3,R)×O($N-1$) spatial wave functions can be combined with the latter to produce totally antisymmetric nuclear shell model states.

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II. REPRESENTATIONS OF Sp(3,R)

A convenient basis for the complexification of sp(3,R) is given by the quadratics

$$\begin{aligned} &A_{ij}=\frac{1}{2}\sum_n a_{in}^\dagger a_{jn}^\dagger, \quad B_{ij}=\frac{1}{2}\sum_n a_{in}a_{jn},\\ &C_{ij}=\frac{1}{2}\sum_n (a_{in}^\dagger a_{jn}+a_{jn}a_{in}^\dagger), \end{aligned} \tag{2}$$

where $(a_{in}^\dagger)$ and (a_{in}) are the harmonic-oscillator step-up and step-down operators for A particles in three dimensions. They satisfy the boson commutation relations

$$\begin{aligned} &[a_{im}^\dagger,a_{jn}^\dagger]=[a_{im},a_{jn}]=0,\\ &[a_{im},a_{jn}^\dagger]=\delta_{ij}\delta_{mn} \end{aligned} \tag{3}$$

and act on $L^2(R^{3A})$

$$\begin{aligned} &\langle x|a_{in}|\Psi\rangle=\frac{1}{\sqrt{2}}\left(x_{in}+\frac{\partial}{\partial x_{in}}\right)\langle x|\Psi\rangle,\\ &\langle x|a_{in}^\dagger|\Psi\rangle=\frac{1}{\sqrt{2}}\left(x_{in}-\frac{\partial}{\partial x_{in}}\right)\langle x|\Psi\rangle, \end{aligned} \tag{4}$$

where $L^2(R^{3A})$ is the space of square integrable functions of the nucleon coordinates $(x_{in};\ i=1,2,3,\ n=1,\ldots,A)$. By putting $A=N-1$, where N is the nucleon number, and by regarding the (x_{in}) as Jacobi relative coordinates, spurious center-of-mass contributions to the collective dynamics are eliminated.

The action of the sp(3,R) Lie algebra implied by Eq. (2) integrates to a unitary action of the Sp(3,R) group.

To construct a unirrep, we seek a lowest weight state Ψ^m (more conventionally called a highest weight state) satisfying

$$B_{ij}|\Psi^m\rangle=0, \quad i,j=1,2,3, \tag{5}$$

$$C_{ij}|\Psi^m\rangle=0, \quad 1\leqslant i\leqslant j\leqslant 3, \tag{6}$$

$$C_{ii}|\Psi^m\rangle=(m_i+A/2)|\Psi^m\rangle, \quad i=1,2,3, \tag{7}$$

where $m=(m_1,m_2,m_3)$, a triple of integers, denotes the number of harmonic-oscillator quanta in the three Cartesian directions. The carrier space $\mathscr{H}^m$ for the above unirrep is then given by

$$\mathscr{H}^m=\mathrm{span}\{\rho(g)|\Psi^m\rangle;\ g\in \mathrm{Sp}(3,R)\}. \tag{8}$$

Observe that Eqs. (6) and (7) also define a lowest weight state for a U(3) unirrep with carrier space

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$$\mathscr{H}_0^m = \text{span}\{\rho(u)|\Psi^m\rangle;\quad u \in \text{U}(3)\}. \tag{9}$$

Evidently we can also identify $\mathscr{H}_0^m$ as the subspace of states in $\mathscr{H}^m$ satisfying Eq. (5). This subspace will be referred to as the U(3) lowest weight space.

Basis states for $\mathscr{H}_0^m$ can be labeled by the U(3) Gel'fand patterns

$$\alpha = \begin{bmatrix} m_1 & m_2 & m_3 \\ & n_1' & n_2' \\ & & n_1'' \end{bmatrix}, \qquad \begin{matrix} m_1 \geqslant n_1' \geqslant m_2 \geqslant n_2' \geqslant n_3, \\ n_1' \geqslant n_1'' \geqslant n_2'. \end{matrix} \tag{10}$$

Such basis states satisfy

$$C_{ii}|\Psi_\alpha^m\rangle = (n_i(\alpha) + A/2)|\Psi_\alpha^m\rangle, \quad i = 1,2,3, \tag{11}$$

where $n_i(\alpha)$, the number of oscillator quanta in the ith Cartesian coordinate direction for the state α, is given by

$$\begin{aligned} &n_1(\alpha) = n_1'', \ n_2(\alpha) = n_1' + n_2' - n_1'', \\ &n_3(\alpha) = m_1 + m_2 + m_3 - n_1' - n_2'. \end{aligned} \tag{12}$$

Basis states for $\mathscr{H}^m$ are obtained by the action of a basis of polynomials in the (A_{ij}) raising operators on the $\mathscr{H}_0^m$ basis.

III. REPRESENTATIONS OF O(A)

The unitary action of the O(A) group on $L^2(R^{3A})$ is defined by

$$[\sigma(t)\Psi](x) = \Psi(xt), \quad t \in O(A). \tag{13}$$

This induces the realization of the o(A) = so(A) Lie algebra

$$\begin{aligned} J_{mn} &= -i\sum_{k=1}^{3}\left(x_{km}\frac{\partial}{\partial x_{kn}} - x_{kn}\frac{\partial}{\partial x_{km}}\right) \\ &= -i\sum_{k=1}^{3}(a_{km}^\dagger a_{kn} - a_{kn}^\dagger a_{km}). \end{aligned} \tag{14}$$

To construct irreducible representations of SO(A), we must first specify a Cartan subalgebra. A convenient choice is the span of the commuting operators

$$H_1 = J_{12},\ H_2 = J_{34},\ldots,\ H_l = J_{A-1,A},\ \text{or}\ J_{A-2,A-1}, \tag{15}$$

where $H_l = J_{A-1,A}$ or $J_{A-2,A-1}$ according as A is even or odd. An irreducible SO(A) representation is then defined by a lowest weight state Ψ and the corresponding l-tuple of eigenvalues $f = (m_1,m_2,\ldots,m_l)$, where

$$H_k|\Psi\rangle = m_k|\Psi\rangle, \quad k = 1,\ldots,l. \tag{16}$$

To explicitly construct a lowest weight state, it is convenient to first introduce the elementary functions[5]

$$\begin{aligned} &\phi_1(X) = X_1 + iX_2, \\ &\phi_2(X) = X_3 + iX_4, \text{ etc.}, \end{aligned} \tag{17}$$

where we use the notation

$$(X_n, Y_n, Z_n) = (x_{1n}, x_{2n}, x_{3n}). \tag{18}$$

These functions evidently have weights (1,0,...,0), (0,1,0,...,0), etc., respectively, and serve as building blocks for lowest weight states. One sees that, for $A \geqslant 6$, the square integrable functions

$$\Psi^m(x) = e^{-(1/2)R^2}P^m(x), \tag{19}$$

where R^2 is the O(A) scalar $R^2 = \Sigma_{in}x_{in}^2$, and

$$\begin{aligned} P^m(x) = [\phi_1(X)]^{\lambda_1}&\begin{bmatrix}\phi_1(X) & \phi_1(Y)\\ \phi_2(X) & \phi_2(Y)\end{bmatrix}^{\lambda_2} \\ \times&\begin{bmatrix}\phi_1(X) & \phi_1(Y) & \phi_1(Z)\\ \phi_2(X) & \phi_2(Y) & \phi_2(Z)\\ \phi_3(X) & \phi_3(Y) & \phi_3(Z)\end{bmatrix}^{\lambda_3} \end{aligned} \tag{20}$$

with $\lambda_i \geqslant 0$, are highest weight states; i.e., lowest with respect to a reverse ordering of the Cartan operators, Eq. (15). Thus P^m defines an SO(A) representation

$$f = (m_1, m_2, m_3, 0,\ldots,0). \tag{21}$$

It is known that the only SO(A) representations that occur in $L^2(R^{3A})$ are of the type (21) with m_1, m_2, m_3 taking integer values.[6,7]

In fact, we need to consider O(A) rather than SO(A) because only O(A) contains the symmetric group S_N ($N = A + 1$) as a subgroup. Now, when A is odd, the representation spaces for O(A) and SO(A) are the same.[7] But, when A is even, an O(A) representation space, in general, contains a conjugate pair of SO(A) representations $(m_1, m_2, \ldots, m_l)$ and $(m_1, m_2, \ldots, -m_l)$ with $m_1 \geqslant m_2 \geqslant \cdots \geqslant m_l \geqslant 0$. However, for the representations occurring in $L^2(R^{3A})$ this extra complication does not arise provided $A \geqslant 7$, for then A is odd or $m_l = 0$.

Since the above Sp(3,R) and O(A) operators commute, states in $L^2(R^{3A})$ can be labeled according to their transformation properties under both groups. Now it is known that the decomposition of $L^2(R^{3A})$ into irreducible Sp(3,R)$\times$O(A) subspaces has two important properties. Firstly, the decomposition is multiplicity free and secondly, the two subgroups Sp(3,R) and O(A) are complementary in that a unique representation $f = (m_1,m_2,m_3,0,\ldots,0)$ of O(A) occurs in combination with the Sp(3,R) representation $m = (m_1,m_2,m_3)^3$. Thus a single label m serves to label unireps of the direct product group Sp(3,R)$\times$O(A). In an obvious extension of the definitions (8) and (9) of $\mathscr{H}^m$ and $\mathscr{H}_0^m$ we now define H^m to be the carrier space for the Sp(3,R)$\times$O(A) unirrep m and H_0^m to be the carrier space for the corresponding lowest weight U(3)$\times$O(A) unirrep space.

As a consequence of the above, basis states for H^m can be constructed with labels λ and ν, where λ indexes an Sp(3,R) basis, constructed as indicated in Sec. II and

$$\nu = \begin{bmatrix} m_1 & m_2 & m_3 & 0 & \cdots & 0 \\ m_1' & m_2' & m_3' & 0 & \cdots & \\ m_1'' & m_2'' & m_3'' & 0 & \cdots & \\ & & \cdots & & & \\ & & \cdots & & & \\ & & m_1^{(A-1)} & & & \end{bmatrix} \tag{22}$$

indexes an SO(A) Gel'fand basis. Similarly, a basis for H_0^m can be constructed with labels α and ν, where α indexes a U(3) Gel'fand basis Eq. (10) and ν is again given by Eq. (22).

Wave functions of $L^2(R^{3A})$ are customarily expressed in the form

$$\Psi(x) = e^{-R^2/2}P(x), \tag{23}$$

where $R^2 = \Sigma_{in}x_{in}^2$ and, in a harmonic-oscillator basis, $P(x)$ is a polynomial. Since

$$\frac{\partial \Psi}{\partial x_{in}}(x) = e^{-(1/2)R^2}\left(\frac{\partial}{\partial x_{in}} - x_{in}\right)P(x), \tag{24}$$

it follows, from Eqs. (2) and (4) that

$$A_{ij}\Psi(x) = e^{-(1/2)R^2}\sum_n\left(x_{in} - \frac{1}{2}\frac{\partial}{\partial x_{in}}\right) \times\left(x_{jn} - \frac{1}{2}\frac{\partial}{\partial x_{jn}}\right)P(x),$$

$$B_{ij}\Psi(x) = e^{-(1/2)R^2}\frac{1}{4}\sum_n \frac{\partial^2}{\partial x_{in}\partial x_{jn}}P(x), \tag{25}$$

$$C_{ij}\Psi(x) = e^{-(1/2)R^2}\left(\sum_n\left(x_{in} - \frac{1}{2}\frac{\partial}{\partial x_{in}}\right)\frac{\partial}{\partial x_{jn}} + \delta_{ij}\frac{A}{2}\right)P(x).$$

Introducing the Laplacian

$$\Delta = \sum_{in}\frac{\partial^2}{\partial x_{in}^2} \tag{26}$$

and observing that

$$e^{-\Delta/4}x_{in}e^{\Delta/4} = x_{in} - \frac{1}{2}\frac{\partial}{\partial x_{in}}, \tag{27}$$

Eq. (25) becomes

$$A_{ij}\Psi(x) = e^{-(1/2)R^2}e^{-\Delta/4}Q_{ij}e^{\Delta/4}P(x), \tag{28a}$$

$$B_{ij}\Psi(x) = e^{-(1/2)R^2}e^{-\Delta/4}\frac{1}{4}\sum_n\frac{\partial^2}{\partial x_{in}\partial x_{jn}}e^{\Delta/4}P(x), \tag{28b}$$

$$C_{ij}\Psi(x) = e^{-(1/2)R^2}e^{-\Delta/4}(E_{ij} + \delta_{ij}A/2)e^{\Delta/4}P(x), \tag{28c}$$

where Q_{ij} is the Cartesian quadrupole moment

$$Q_{ij} = \sum_n x_{in}x_{jn} \tag{29}$$

and

$$E_{ij} = \sum_n x_{ni}\frac{\partial}{\partial x_{nj}} \tag{30}$$

is an element of gl(3,R), the Lie algebra of the general linear group in three dimensions. Equation (28c) is simply an expression of the well-known isomorphism between gl(3,R) and the complexified u(3) Lie algebra.

Now, if Ψ is in the U(3) lowest weight space $\mathscr{H}_0^m$ Eq. (9), then $B_{ij}\Psi = 0$ and, by Eq. (28b),

$$\sum_n \frac{\partial^2}{\partial x_{in}\partial x_{jn}}P(x) = 0. \tag{31}$$

Hence, $\Delta P(x) = 0$ and

$$e^{\Delta/4}P(x) = P(x). \tag{32}$$

It follows from these equations and Eq. (28c) that the polynomials $P(x)$ corresponding to states in the U(3) representation space $\mathscr{H}_0^m$ are harmonic and homogeneous of degree $m_1 + m_2 + m_3$ and carry an irreducible (nonunitary) representation (m_1,m_2,m_3) of $GL_+(3,R)$. Thus we may define a basis of harmonic homogeneous polynomials $\{P_{\alpha\nu}^m\}$ for an irreducible representation of $GL_+(3,R)\times O(A)$, with α indexing a $GL_+(3,R)$ Gel'fand basis and ν indexing an $SO(A)$ Gel'fand basis. Then, from the definition, Eqs. (10) and (11) of the u(3)$\sim$gl(3,R) Gel'fand basis, we have

$$E_{ii}P_{\alpha\nu}^m(x) = n_i(\alpha)P_{\alpha\nu}^m(x), \tag{33}$$

and the corresponding states $\{\psi_{\alpha\nu}^m\}$ carry a unirrep m of $U(3)\times O(A)$ and provide a basis for H_0^m.

The construction of these polynomials is discussed in the following section. In concluding this section, we remark only that, to augment the $U(3)\times O(A)$ representation space H_0^m to the representation space H^m for $Sp(3,R)\times O(A)$, we have simply to apply the sp(3,R) raising operators (A_{ij}) repeatedly to each of the $\{\psi_{\alpha\nu}^m\}$ basis states. Then, using Eq. (28a), we note that

$$[A_{ij}\times\cdots\times A_{lk}]\psi_{\alpha\nu}^m(x) = e^{-(1/2)R^2}e^{-\Delta/4}[Q_{ij}\times\cdots\times Q_{lk}]P_{\alpha\nu}^m(x). \tag{34}$$

Thus, it follows that a basis of polynomials for H^m can be constructed of the form $\{F_\sigma(Q)P_{\alpha\nu}^m(x)\}$, where $\{F_\sigma(Q)\}$ are polynomials in the $\{Q_{ij}\}$.

IV. POLYNOMIALS FOR H_0^m

We wish to construct the harmonic homogeneous polynomials $\{P_{\alpha\nu}^m\}$ on R^{3A} that carry a left representation (m_1,m_2,m_3) of $GL_+(3,R)$ and a right representation $(m_1,m_2,m_3,0,\ldots,0)$ of $O(A)$. Thus we want polynomials satisfying

$$P_{\alpha\nu}^m(gx) = \sum_{\beta=1}^{d_1}\Gamma_{\alpha\beta}^m(g)P_{\beta\nu}^m(x), \quad g\in GL_+(3,R), \tag{35}$$

$$P_{\alpha\nu}^m(xc) = \sum_{\mu=1}^{d_2}P_{\alpha\mu}^m(x)D_{\mu\nu}^m(c), \quad c\in O(A), \tag{36}$$

where Γ^m and D^m are, respectively, the representation matrices for $GL_+(3,R)$ and $O(A)$. Note that the required representation for $GL_+(3,R)$, being of finite dimension d_1 is not unitary.

Now any $x\in R^{3A}$ can be factored

$$x = bEc, \tag{37}$$

where b is a positive symmetric 3×3 matrix defined by $b^2 = x\tilde{x}$, E is the $3\times A$ matrix

$$E_{\alpha\nu} = \delta_{\alpha\nu}, \tag{38}$$

and $c\in O(A)$. It follows that, with this factorization,

$$P_{\alpha\nu}^m(x) = \sum_{\beta=1}^{d_1}\sum_{\mu=1}^{d_2}\Gamma_{\alpha\beta}^m(b)P_{\beta\mu}^m(E)D_{\mu\nu}^m(c). \tag{39}$$

Thus to discover the general form of a polynomial $P_{\alpha\nu}^m$, we need to consider the three factors in this equation.

Consider first the $GL_+(3,R)$ matrix $\Gamma^m(d)$ for d a diagonal matrix $d = \mathrm{diag}(d_1,d_2,d_3)$. From Eq. (33), it follows that

$$\Gamma_{\alpha\beta}^m(d) = \delta_{\alpha\beta}f_\alpha^m(d) \tag{40}$$

with

$$f_\alpha^m(d) = d_1^{n_1(\alpha)}d_2^{n_2(\alpha)}d_3^{n_3(\alpha)}. \tag{41}$$

Since any general linear matrix g can be factored $g = r_1 dr_2$ with r_1 and r_2 rotations, it remains to consider $\Gamma_{\alpha\beta}^m(r)$ for $r\in SO(3)$. Let $C(\delta LM;m\alpha)$ be the linear transformation from the $GL_+(3,R)$ Gel'fand basis to a $GL_+(3,R)\supset SO(3)\supset SO(2)$ basis and let $C(m\alpha;\delta LM)$ be the inverse transformation, where δ is a multiplicity index. It then follows that for $r\in SO(3)$

$$\Gamma^m_{\alpha\beta}(r) = \sum_{\delta LM} C(m\alpha;\delta LM)\mathscr{D}^L_{MN}(r)C(\delta LN;m\beta), \quad (42)$$

where $\mathscr{D}^L$ is a Wigner rotation matrix.

For arbitrary $g = r_1\, dr_2 \in \mathrm{GL}_+(3,R)$, $\Gamma^m(g)$ is evidently given in a $\mathrm{GL}_+(3,R)\supset\mathrm{SO}(3)\supset\mathrm{SO}(2)$ basis by

$$\Gamma^m_{\delta LM,\delta' L'M'}(g) = \sum_{NN'} \mathscr{D}^L_{MN}(r_1)\Gamma^m_{\delta LN,\delta' L'N'}(d)\mathscr{D}^{L'}_{N'M'}(r_2), \quad (43)$$

where

$$\Gamma^m_{\delta LN,\delta' L'N'}(d) = \sum_\alpha C(\delta LN;m\alpha) f^m_\alpha(d) C(m\alpha;\delta' L'N'). \quad (44)$$

Consider next the $d_1\times d_2$ matrix $\{P^m_{\alpha\nu}(E)\}$ and recall that ν indexes an $\mathrm{SO}(A)$ Gel'fand basis Eq. (22). It will be supposed that this basis is ordered such that the first d_1 vectors correspond to patterns of the type

$$\nu = \begin{bmatrix} m_1 & m_2 & m_3 & 0 & \cdots & 0 \\ m_1' & m_2' & 0 & \cdots & 0 & \\ m_1'' & 0 & \cdots & 0 & & \\ 0 & \cdots & 0 & & & \\ \cdots & & & & & \\ 0 & & & & & \end{bmatrix}, \quad 1\leqslant\nu\leqslant d_1. \quad (45)$$

One observes that there are indeed just d_1 such Gel'fand patterns since they are in one-to-one correspondence with the U(3) or $\mathrm{GL}_+(3,R)$ patterns of Eq. (10). Observe too that the corresponding basis vectors are all $\mathrm{O}(A-3)$ invariant and in fact span the maximal $\mathrm{O}(A-3)$ invariant subspace of the full $\mathrm{O}(A)$ representation space.

The construction of the required polynomials is now facilitated by use of the following theorems proved in the Appendix.

Theorem 1: If V^m is the carrier space for an irreducible representation $(m_1,m_2,m_3,0,\ldots,0)$ of $\mathrm{O}(A)$, then the maximal $\mathrm{O}(A-3)$ invariant subspace V^m_0 of V^m carries an irreducible tensor representation (m_1,m_2,m_3) of $\mathrm{GL}_+(3,R)$.

Theorem 2: In the above ordered basis, $P^m_{\alpha\nu}(E) = 0$ for $\nu > d_1$ and the $d_1\times d_1$ submatrix $(P^m_{\alpha\beta}(E);\alpha\beta = 1,\ldots,d_1)$ is a linear transformation from the $\mathrm{O}(A)$ Gel'fand basis Eq. (45), for V^m_0 to the $\mathrm{GL}_+(3,R)$ Gel'fand basis.

From these theorems, it follows immediately that a basis of polynomials is given, in the $\mathrm{GL}_+(3,R)\supset\mathrm{SO}(3)\supset\mathrm{SO}(2)$ and $\mathrm{O}(A)$ Gel'fand bases, by

$$P^m_{\delta LM\nu}(x) = \sum_{\delta' L'M'\beta} \Gamma^m_{\delta LM,\delta' L'M'}(b)\overline{C}(\delta' L'M';m\beta)D^m_{\beta\nu}(c), \quad (46)$$

where Γ^m is given by Eq. (43) and

$$\overline{C}(\delta LM;m\beta) = \sum_{\alpha=1}^{d_1} C(\delta LM;m\alpha)P^m_{\alpha\beta}(E) \quad (47)$$

is the linear transformation from the $\mathrm{O}(A)$ Gel'fand basis for V^m_0 to the $\mathrm{GL}_+(3,R)\supset\mathrm{SO}(3)\supset\mathrm{SO}(2)$ basis.

V. AN Sp(3,R)×O(A) BASIS FOR THE SHELL MODEL

We now have, from Eq. (46), a basis for the $\mathrm{U}(3)\times\mathrm{O}(A)$ space H^m_0

$$\Psi^m_{\delta LM\nu}(x) = e^{-(1/2)R^2}P^m_{\delta LM\nu}(x). \quad (48)$$

It can be augmented to a basis for the $\mathrm{Sp}(3,R)\times\mathrm{O}(A)$ representation space H^m by multiplying each basis state in H^m_0 by a complete set of polynomials in the symmetric tensor $Q(x) = x\tilde{x}$ as noted in Sec. IV.

Now the matrix elements $\Gamma^{(2,0,0)}_{LM,L'M'}(g)$ of the (2,0,0) representation of $\mathrm{GL}_+(3,R)$ are expressible

$$\Gamma^{(2,0,0)}_{LM,L'M'}(g) = \sum_{\alpha+\beta=M}\sum_{\gamma+\delta=M'} \times(11\alpha\beta|LM)(11\gamma\delta|L'M')g_{\alpha\gamma}g_{\beta\delta}, \quad (49)$$

where $(g_{\alpha\beta})$ are the components of $g\in\mathrm{GL}_+(3,R)$ in the spherical coordinate system and $(11\alpha\beta|LM)$ is an SO(3) Clebsch–Gordan coefficient. For $L = 2$ and $L' = 0$, Eq. (49) becomes

$$\Gamma^{(2,0,0)}_{2M,00}(g) = \frac{1}{5^{1/2}}\sum_{\alpha+\beta=M}(11\alpha\beta|2M)\sum_\nu(-1)^\nu g_{\alpha\nu}g_{\beta-\nu}. \quad (50)$$

For $L = L' = 0$, Eq. (49) becomes

$$\Gamma^{(2,0,0)}_{00,00}(g) = \frac{1}{5}\sum_{\alpha\beta}(-1)^{\alpha+\beta}g_{\alpha\beta}g_{-\alpha,-\beta}. \quad (51)$$

For any $x\in R^{3A}$ we can set $g = b$ in Eqs. (50) and (51), where b is the symmetric 3×3 matrix for which $b^2 = x\tilde{x}$, and obtain

$$\Gamma^{(2,0,0)}_{2M,00}(b)\propto Q_{2M}(x),$$
$$\Gamma^{(2,0,0)}_{00,00}(b)\propto Q_{00}(x), \quad (52)$$

i.e., the quadrupole and monopole moments, respectively. It follows that a basis of polynomials in $Q(x)$ is given by $\{\Gamma^n_{\delta LM,00}(b)\}$, where $n = (n_1,n_2,n_3)$ is a $\mathrm{GL}_+(3,R)$ representation realizable as a symmetric product of (2,0,0) representations. The n-representations realizable in this way are well known and are given by the set of all even integers n_1,n_2,n_3 satisfying the inequality

$$n_1\geqslant n_2\geqslant n_3\geqslant 0. \quad (53)$$

Thus a basis for H^m is given by the set of wave functions

$$\Psi^m_{\delta_1L_1M_1\delta_2L_2M_2\nu}(x) = e^{-(1/2)R^2}e^{-\Delta/4}\Gamma^n_{\delta_1L_1M_1,00}(b)P^m_{\delta_2L_2M_2\nu}(x), \quad (54)$$

where Δ is the Laplacian Eq. (26), Γ^n is defined by Eq. (43) and P^m by Eq. (46). This basis can evidently be coupled to good $\mathrm{U}(3)\supset\mathrm{SO}(3)$ symmetry in an obvious way.

Finally, note that H^m is not a shell model Hilbert space. The shell model space is the space of totally antisymmetric combinations of $L^2(R^{3A})$ spatial wave functions and spin-isospin wave functions. To obtain a shell model basis for a unirrep m of $\mathrm{Sp}(3,R)$, we must therefore, first transform the above $\mathrm{SO}(A)$ Gel'fand basis to a $\mathrm{O}(A)\supset S_N$ basis, where S_N is the symmetric group for $N = A+1$ nucleons.

Let $K(m\nu;\epsilon[f]\sigma)$ denote a transformation coefficient for the above change of basis, where $[f]$ labels a S_N unirrep, σ a basis for this representation, and ϵ is a multiplicity index. We can now define the fully antisymmetric functions

$$\mathbb{P}^{m\epsilon[f]}_{\delta LM}(x) = \sum_{\nu\sigma}P^m_{\delta LM\nu}(x)K(m\nu;\epsilon[f]\sigma)X^{[\tilde{f}]}_\sigma, \quad (55)$$

where $\{X^{[\tilde{f}]}_\sigma\}$ is a basis of spin-isospin wave functions for a representation $[\tilde{f}]$ of S_N contragredient to $[f]$.

Thus, we obtain a shell model basis for an Sp(3,R) unirrep m

$$\phi^{m\epsilon[f]}_{n\delta_1 L_1 M_1 \delta_2 L_2 M_2}(x) = e^{-(1/2)R^2} e^{-\Delta/4} \Gamma^n_{\delta_1 L_1 M_1, 0}(b)\, \mathbb{P}^{m\epsilon[f]}_{\delta_2 L_2 M_2}(x). \tag{56}$$

VI. SUMMARY

In summary, we have found an Sp(3,R)$\times$O(A) basis of wave functions

$$\phi^{m\epsilon[f]}_{n\delta_1 L_1 M_1 \delta_2 L_2 M_2}(x) = e^{-(1/2)R^2} e^{-\Delta/4} \Gamma^n_{\delta_1 L_1 M_1, 00}(b)\, \mathbb{P}^{m\epsilon[f]}_{\delta_2 L_2 M_2}(x) \tag{57}$$

for the nuclear shell model, where Γ^n is a GL$_+$(3,R) representation matrix, in a GL$_+$(3,R)$\supset$SO(3)$\supset$SO(2) basis, given explicitly in Eq. (43), b is the symmetric 3×3 matrix defined by $b^2 = x\tilde{x}$ and

$$\mathbb{P}^{m\epsilon[f]}_{\delta L M}(x) = \sum_{\delta' L' M' \kappa} \Gamma^m_{\delta L M, \delta' L' M'}(b) \times \langle m\delta' L' M' | \sigma(c) | m\epsilon[f]\kappa \rangle X^{[\tilde{f}]}_{\kappa}, \quad x = bEc, \quad c \in O(A). \tag{58}$$

Note that the second factor on the right of Eq. (58) is an O(A) matrix element between an O(A)$\supset S_N$ basis state on the right and a GL$_+$(3,R)$\supset$SO(3)$\supset$SO(2) basis state for the O($A-3$) invariant subspace of the O(A) m-representation space on the left. It was related previously to the O(A) matrix elements $D^m_{\beta\nu}(c)$, in a Gel'fand basis, by

$$\langle m\delta' L' M' | \sigma(c) | m\epsilon[f]\kappa \rangle = \sum_{\beta\nu} \overline{C}(\delta' L' M'; m\beta) D^m_{\beta\nu}(c) K(m\nu; \epsilon[f]\kappa), \tag{59}$$

where $\overline{C}$ and K are the linear transformations of the basis. The third factor $X^{[\tilde{f}]}_{\kappa}$ in Eq. (58) is a spin-isospin wave function of symmetry $[\tilde{f}]$ contragredient to the symmetry $[f]$ of the spatial wave function so that the combination is fully antisymmetric.

In practical applications, it is convenient to work with a basis of shell model wave functions that reduce the subgroup chain

$$\mathrm{Sp}(3,R)\supset \mathrm{U}(3)\supset \mathrm{SU}(3)\supset \mathrm{SO}(3)\supset \mathrm{SO}(2). \tag{60}$$

Such a basis is now obtained simply by the unitary transformation

$$\phi^{m\epsilon[f]}_{n(\lambda\mu)\delta L M} = \sum_{\delta_1 L_1 M_1 \delta_2 L_2 M_2} \langle (\lambda_n \mu_n)\delta_1 L_1 M_1; (\lambda_m \mu_m)\delta_2 L_2 M_2 | \times \rho(\lambda\mu)\delta L M \rangle \phi^{m\epsilon[f]}_{\rho n \delta_1 L_1 M_1 \delta_2 L_2 M_2}, \tag{61}$$

where

$$\lambda_n = n_1 - n_2, \quad \mu_n = n_2 - n_3, \tag{62}$$

the transformation coefficient is an SU(3) Clebsch–Gordan coefficient, and ρ is a multiplicity index.

In order to assist in the interpretation of the collective content of microscopic shell model wave functions we would further like to discover the transformation coefficients between the basis states of the subgroup chain (60) and those of the chain

$$\mathrm{Sp}(3,R)\supset CM(3)\supset \mathrm{SO}(3)\supset \mathrm{SO}(2). \tag{63}$$

However, we have not yet succeeded in finding them.

Note added in proof: Subsequent to submission of this manuscript, one of us has developed recursion relations for the overlaps of the above basis states, using coherent state theory, and shown how to transform them into an orthonormal basis and calculate Sp(3,R) matrix elements [D. J. Rowe, J. Math. Phys. **25**, 2662 (1984)].

ACKNOWLEDGMENT

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada.

APPENDIX

Theorem 1: If V^m is the carrier space for an irreducible representation $(m_1,m_2,m_3,0,\ldots,0)$ of O(A), then the maximal O($A-3$) invariant subspace V^m_0 of V^m carries an irreducible tensor representation (m_1,m_2,m_3) of GL$_+$(3,R). To prove this theorem we need the following propositions.

Proposition 1: If $g \in$ GL(3,R), there exists some $G \in$ O(A) of the block form

$$G = \frac{1}{k}\begin{bmatrix} g & A \\ B & C \end{bmatrix}, \tag{A1}$$

where k is a positive number.

Proof: The proposition is obviously true if $g \in$ O(3) with $k=1$, $A=B=0$, and $C = I_{A-3}$. Thus, since any $g \in$ GL(3,R) can be factored $g = r_1 d r_2$, where $r_1, r_2 \in$ O(3) and d is diagonal with entries $d_1 \geqslant d_2 \geqslant d_3 > 0$, it is sufficient to consider such diagonal matrices. For $g = d$, one can evidently construct an O(A) matrix

$$G = \frac{1}{d_1}\begin{pmatrix} d_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & (d_1^2 - d_2^2)^{1/2} & 0 & 0 \\ 0 & 0 & d_3 & 0 & (d_1^2 - d_3^2)^{1/2} & 0 \\ 0 & -(d_1^2 - d_2^2)^{1/2} & 0 & d_2 & 0 & 0 \\ 0 & 0 & -(d_1^2 - d_3^2)^{1/2} & 0 & d_3 & 0 \\ 0 & 0 & 0 & 0 & 0 & I \end{pmatrix} \tag{A2}$$

which completes the proof. □

Proposition 2: The dimension of V^m_0 is equal to the dimension d_1 of the GL$_+$(3,R) representation (m_1,m_2,m_3).

Proof: Construct an ordered basis for V^m such that the first d_1 basis vectors correspond to O(A) Gel'fand patterns of the type shown in Eq. (45). These are O($A-3$) invariant and span the O($A-3$) invariant subspace V^m_0. Now observe that these patterns are in one-to-one correspondence with the GL$_+$(3,R) Gel'fand patterns of Eq. (10). □

Proposition 3: In the above ordered basis, the $d_1\times d_1$ submatrix T of the matrix

$$D^m(G) = \begin{pmatrix} T & X \\ Y & Z \end{pmatrix} \tag{A3}$$

for the O(A) representation $(m_1,m_2,m_3,0,\ldots,0)$ depends only on the elements of the 3×3 submatrix a of the O(A) matrix

$$G=\begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{A4}$$

Proof: Define $S(a)$ to be the set of all $O(A)$ matrices with left upper 3×3 submatrix equal to a; i.e.,

$$S(a)=\left\{G\in O(A);\ G=\begin{pmatrix} a & * \\ * & * \end{pmatrix}\right\}. \tag{A5}$$

Evidently $S(a)$ is invariant under both left and right multiplication by a group element

$$h=\begin{pmatrix} I_3 & 0 \\ 0 & u \end{pmatrix},\quad u\in O(A-3). \tag{A6}$$

Thus $S(a)$ is a double coset in the double factor space $O(A-3)\backslash O(A)/O(A-3)$. Now $D^m(h)$ is of block form

$$D^m(h)=\begin{pmatrix} I_{d_1} & 0 \\ 0 & W \end{pmatrix}. \tag{A7}$$

It follows that

$$T(hG)=T(Gh)=T(G). \tag{A8}$$

In other words, T is a function only of the double coset $S(a)$. □

Proposition 4: The polynomials $\{P^m_{\alpha\nu};\alpha=1,\ldots,d_1,\nu=1,\ldots,d_2\}$ on R^{3A} that carry a left representation (m_1,m_2,m_3) of $GL_+(3,R)$ and a right representation $(m_1,m_2,m_3,0,\ldots,0)$ of $O(A)$ have the property that, in the above ordered basis,

$$P^m_{\alpha\nu}(E)=0 \quad \text{if } \nu>d_1, \tag{A9}$$

where $E\in R^{3A}$ is defined by Eq. (38).

Proof: Observe that E is $O(A-3)$ invariant; i.e., for $h\in O(A)$ given by Eq. (A6), $Eh=E$. Furthermore, in the ordered basis, $D^m(h)$ is of block form (A7). Thus,

$$P^m_{\alpha\nu}(Eh)=\sum_{\mu}P^m_{\alpha\mu}(E)D^m_{\mu\nu}(h)=P^m_{\alpha\nu}(E) \tag{A10}$$

for any $u\in O(A-3)$, implying Eq. (A9). □

Proposition 5: The $d_1\times d_1$ matrix $[P^m_{\alpha\beta}(E);\alpha,\beta=1,\ldots,d_1]$ is nonsingular.

Proof: By Proposition 4

$$P^m_{\alpha\gamma}(EG)=\sum_{\beta=1}^{d_1}P^m_{\alpha\beta}(E)D^m_{\beta\gamma}(G). \tag{A11}$$

It follows, by Proposition 3, that, for $\gamma\leqslant d_1$, $P^m_{\alpha\gamma}(EG)$ is a function only of $k^{-1}g$ and that

$$P^m_{\alpha\gamma}(gE)=P^m_{\alpha\gamma}(kEG)=\sum_{\beta=1}^{d_1}P^m_{\alpha\beta}(kE)D^m_{\beta\gamma}(G). \tag{A12}$$

Now $(P^m_{\alpha\beta}(E))$ singular means that there exist some numbers (λ_α) such that $\Sigma_\alpha\lambda_\alpha P^m_{\alpha\beta}(E)=0$ which, since the $\{P^m_{\alpha\nu}\}$ are all homogeneous of constant degree, means $\Sigma_\alpha\lambda_\alpha P^m_{\alpha\beta}(kE)=0$, which in turn, by Eq. (A12), means $\Sigma_\alpha\lambda_\alpha P^m_{\alpha\gamma}(gE)=0$ and

$$\sum_{\alpha,\beta}\lambda_\alpha P^m_{\alpha\gamma}(gE)D^m_{\gamma\nu}(c)=\sum_{\alpha}\lambda_\alpha P^m_{\alpha\nu}(gEc)=0 \tag{A13}$$

for any $c\in O(A)$. Since almost any $x\in R^{3A}$ can be expressed as a product $x=gEc$ for some $g\in GL_+(3,R)$, $c\in O(A)$, it follows that $(P^m_{\alpha\beta}(E))$ singular implies $\Sigma_\alpha\lambda_\alpha P^m_{\alpha\nu}(x)=0$ for any $x\in R^{3A}$. But this is impossible because the polynomials $\{P^m_{\alpha\nu}\}$ are a basis for an irreducible representation of the group $GL_+(3,R)\times O(A)$ and must, therefore, be linearly independent. □

Proof of Theorem 1: Since the elements of $D^m(G)$ are homogeneous polynomials of degree $(m_1+m_2+m_3)$ in the elements of G, it follows, by Propositions 1 and 3 that we can define the $d_1\times d_1$ array of functions of $GL_+(3,R)$

$$T^m_{\alpha\beta}(g)=k^{m_1+m_2+m_3}D^m_{\alpha\beta}(G),\quad \alpha,\beta=1,\ldots,d_1. \tag{A14}$$

The identity $P^m_{\alpha\gamma}(gE)=P^m_{\alpha\gamma}(kEG)$, for $\gamma\leqslant d_1$, now implies

$$\sum_{\beta}\Gamma^m_{\alpha\beta}(g)P^m_{\beta\gamma}(E)=\sum_{\beta}P^m_{\alpha\beta}(E)T^m_{\beta\gamma}(g). \tag{A15}$$

Since $(P^m_{\alpha\beta}(E))$ is nonsingular, this equation means that T^m is a representation of $GL_+(3,R)$ equivalent to the irreducible representation Γ^m and that $(P^m_{\alpha\beta}(E))$ is the intertwining operator. □

Theorem 2: In the above ordered basis, $P^m_{\alpha\nu}(E)=0$ for $\nu>d_1$ and the $d_1\times d_1$ submatrix $(P^m_{\alpha\beta}(E);\alpha,\beta=1,\ldots,d_1)$ is a linear transformation from the $O(A)$ Gel'fand basis for V^m_0 to the $GL_+(3,R)$ Gel'fand basis.

Proof: This theorem follows immediately from Proposition 4 and Eq. (A15) and the fact that Γ^m was defined as the representation of $GL_+(3,R)$ in a $GL_+(3,R)$ Gel'fand basis. □

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Electrons moving in a crystal weakly coupled to a random reservoir

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(Received 3 February 1984; accepted for publication 4 May 1984)

We present here an illustration of the difference between static and temporal disorders. We consider a model which is modification of one previously introduced by Martin and Emch, to discuss the mechanism of the long-time, weak-coupling limit in statistical mechanics. It consists of an electron moving in a crystal where impurities are randomly scattered. We introduce a stochastic time disorder in the potential and prove that this new stochastic dynamics converges to a semigroup law without the limitations occurring in the work of Martin and Emch, i.e., the short time restriction and in any space dimension.

PACS numbers: 72.10.Fk, 02.50.Ey

I. INTRODUCTION

We here construct a Hamiltonian model for which we can prove the existence of the so-called Van Hove's long-time, weak-coupling limit.[1] Our system will be described by a time-dependent Hamiltonian of the form

$$H(t) = H_0 + \lambda V(t).$$

The free Hamiltonian H_0 is diagonal in the momentum representation. λ is a dimensionless parameter which measures the strength of the interaction. $V(t)$ is a potential random in time and space defined by a multidimensional stationary Gaussian process $v_n(t)$, $n \in \mathbb{Z}^3$, $t \geqslant 0$, with zero mean, and time-dependent correlation functions given by

$$\langle v_n(t) v_m(s) \rangle = g_{n-m} e^{-c(t-s)^2},$$

$\forall n,m \in \mathbb{Z}^3$, $s,t \geqslant 0$. The parameter $c > 0$ indicates the random time dependence, in the sense that if $c = 0$, the electron moves in a static random medium.

We are able to prove the convergence of the expected value of this model's wave packet as $\lambda \to 0$ and $\tau = \lambda^2 t$ remains constant, for all rescaled time τ. This result is an improvement on the ones already obtained for other models.

The proof of our result consists of checking the hypotheses of a theorem on asymptotic analysis of random differential equations proved in Ref. 2. This result imposes a strong mixing condition on the model's dynamics.

We were motivated by the work of Martin and Emch,[3] where they constructed the first nontrivial model to show all the phenomenon proposed by Van Hove for which the weak-coupling limit could be controlled rigorously through the perturbation expansion as suggested by Van Hove. The Martin–Emch model consists of an electron moving in a crystal, represented by the lattice $\mathbb{Z}^3$, where impurities are located, and has a Hamiltonian of the form $H_0 + \lambda V$. The potential V is given through a static real Gaussian stochastic process. Martin and Emch successfully obtained from the microscopic dynamics the macroscopic one described by the so-called Master equation. They succeeded in controlling The Dyson expansion series for the solution of the stochastic equation, but a radius of convergence τ_0 appeared. That is, the long-time weak-coupling limit is computed only for $0 \leqslant \tau \leqslant \tau_0$. This restriction is unexpected since it has no physical explanation, although it seems to be a consequence of the method used in their proof. Spohn[4] extended their result for functions of the momentum, but the time restriction still ramained. Also quoted by Martin and Emch and Spohn, as unsatisfactory are (i) the deep dependence of their proofs on the electron-type dispersion law, if this law is slightly altered their proof does not work out; and (ii) the restriction on the dimension of the lattice. We emphasize that our proof has no time restriction, permits the use of other dispersion laws, and holds for models with any finite dimensional lattice.

In this work, we also link our result with the one obtained by Martin and Emch, although their model has a different dynamics. We have introduced an assembly of models indexed by the parameter c, where for each model there is no time restriction on the validity of the result macroscopic equation. We prove that as $c \to 0$ (i.e., as we weaken the medium random time dependence), our macroscopic dynamics converges strongly to the one obtained by Martin and Emch.

II. DESCRIPTION OF THE MODEL

According to the formalisms of Hamiltonian mechanics, our model consists of an electron moving in a crystal weakly coupled to a reservoir that scatters impurities on the crystal.

Our free system is represented by the Hilbert space $\mathscr{H}$, the reservoir is given by the Hilbert space $\mathscr{F}$, and the system plus reservoir by $\mathscr{H} \otimes \mathscr{F}$. The Hamiltonian on $\mathscr{H} \otimes \mathscr{F}$ is

$$H = H_{\mathscr{H}} \otimes I + I \otimes H_{\mathscr{F}} + \lambda H_I,$$

where $H_{\mathscr{H}}$ is the free Hamiltonian, $H_{\mathscr{F}}$ is the reservoir Hamiltonian, λH_I represents the interaction between the two entities, and λ is a dimensionless coupling parameter measuring the strength of the interaction causing collisions.

Here, we work in the same framework used by Emch and Martin[3] (for a more general structure see Ref. 4). We consider $\mathscr{H} = \mathscr{L}^2(\mathbb{Z}^3)$ and $\mathscr{F} = \mathscr{L}^2(\Omega, \mathscr{A}, P)$, where the triple $(\Omega, \mathscr{A}, P)$ is a probability space. The Hamiltonian $H_{\mathscr{H}}$ is defined by its momentum representation in the Hilbert space $\mathscr{L}^2(B)$, where $B = [-\pi, \pi]^3$,

$$(H_{\mathscr{H}} \phi)(\theta) = \theta^2 \phi(\theta),$$

where $\theta = (\theta_1, \theta_2, \theta_3) \in V$, $\theta^2 = \theta_1^2 + \theta_2^2 + \theta_3^2$,

$$\phi(\theta) = \frac{1}{(2\pi)^{3/2}} \sum_{n \in \mathbb{Z}^3} e^{in\theta} \phi_n.$$

 0022-2488/84/123551-07$02.50

The dispersion law $\theta \to \theta^2$ is discussed below.

We introduce the dynamics of the reservoir as one sees it in the Schrödinger picture of the coupled system. We consider a group of measure-preserving transformations $\{T(t): t\in\mathbb{R}\}$ acting in $(\Omega, \mathscr{A}, P)$. Using these transformations, we define a strongly continuous group of unitary operators acting in $\mathscr{F}$:

$$U_{\mathscr{F}}(t); f(\cdot)\in\mathscr{F} \mapsto f(T(t)[\cdot])\in\mathscr{F}.$$

We call $H_{\mathscr{F}}$ the self-adjoint operator which generates the group $U_{\mathscr{F}}(t)$.

The interaction law is given by

$$H_I = \sum_{n\in\mathbb{Z}^3} P_n \otimes Q_n,$$

where $(P_n f)_m = \delta_{nm} f_m$, for every $f\in\mathscr{H}$, $\delta_{nm} = 1$, if $n = m$, and 0, otherwise, and $(Q_n \xi)(\omega) = v_n(\omega)\xi(\omega)$, for every $\xi\in\mathscr{F}$.

As one can see in Ref. 2, the interaction with the reservoir has the effect on the free system of a time-dependent perturbation. The dynamics in $\mathscr{H}$ satisfies the following initial-value problem (for details see Ref. 2):

$$\frac{d\phi_\lambda(t)}{dt} = \lambda V_{\mathscr{H}}(t)\phi_\lambda(t), \quad \phi_\lambda(0) = \phi\in\mathscr{H}, \tag{2.1}$$

where

$$V_{\mathscr{H}}(t) = ie^{-itH_{\mathscr{H}}} \sum_{n\in\mathbb{Z}^3} v_n(T(t)[\cdot])P_n e^{itH_{\mathscr{H}}}. \tag{2.2}$$

We should observe that the operator $V_{\mathscr{H}}(t)$ is unbounded (Theorem 4.1), so we have to prove that (2.1) is well defined for all $\omega\in\Omega$, but a set of measure zero. Because of the unboundedness of $V_{\mathscr{H}}(t)$, Martin and Emch and Spohn[3,4] considered a finite cutoff in the lattice $\mathbb{Z}^3$ and extended the dynamics to the whole $\mathbb{Z}^3$ through an infinite-volume limit. We shall avoid this procedure working with unbounded operators.

We call

$$v_n(t)[\cdot] = v_n(T(t)[\cdot]).$$

The transformations $T(t)$, $t\in\mathbb{R}$, are given by the following conditions:

(i) $E\{v_n(t)\} = 0$,

(ii) $E\{v_n(t)v_m(s)\} = g_{n-m}e^{-c(t-s)^2}$, (2.3)

where c is a positive constant. Here $E\{\cdot\}$ stands for the integration over Ω with respect to P. The constant c will work as a (fixed) parameter through our entire analysis. This means that for each c we have a distinct model, as c gets smaller each system becomes a weaker modification of the so-called Martin–Emch model.[3] The term "weaker modification" will be fully understood later.

The g_n's satisfy the following conditions:

(i) $g_n = g_{-n}$,

(ii) $\|g\|_1 = \sum_{n\in\mathbb{Z}^3} |g_n| < \infty$, (2.4)

(iii) $g(\theta) = \frac{1}{(2\pi)^{3/2}} \sum_{n\in\mathbb{Z}^3} g_n e^{in\theta} > 0$, for every $\theta\in B$.

It is clear that g is a continuous function.

III. ASYMPTOTIC ANALYSIS

We want to show that the system described in Sec. II fulfills all the conditions imposed by the theorem proved in Ref. 2.

We say that W is a random operator acting in $\mathscr{H}$ when for each $\phi\in\mathscr{H}$ there exists a set Ω_ϕ of full measure, such that

$$W(\omega)\phi\in\mathscr{H},$$

for every $\omega\in\Omega_\phi$.

We first prove that Eq. (2.1), which describes the dynamics of the system, makes sense. This means that, for each $t\in\mathbb{R}$, $V_{\mathscr{H}}(t)$ (2.2) is a random operator acting in $\mathscr{H}$ in the sense given above.

Lemma 3.1: For every $\phi\in\mathscr{H}$,

$$V\phi = \sum_{n\in\mathbb{Z}^3} v_n P_n \phi \quad \text{a.e.}$$

is a well-defined random vector in $\mathscr{H}$.

Proof: Let $\phi\in\mathscr{H}$ be fixed.

From (2.4), it follows that

$$E\{\|V\phi\|^2\} = g_0\|\phi\|^2.$$

Thus there exists $\Omega_\phi\in\mathscr{A}$, such that $P(\Omega_\phi) = 1$, and for all $\omega\in\Omega_\phi$

$$V(\omega)\phi\in\mathscr{H}. \qquad \square$$

Next we show that the abstract framework of the model discussed in Sec. II satisfies the conditions imposed by the limit theorem in Ref. 2. We start proving that condition (B) of Sec. 2 (in Ref. 2) is satisfied.

Lemma 3.2: There exists a positive constant C such that for every ϕ in $\mathscr{H}$ and $0\leqslant r\leqslant s\leqslant t$:

(i) $E\|V_{\mathscr{H}}(t)\phi\|^2 \leqslant C^2\|\phi\|^2$,

(ii) $E\|V_{\mathscr{H}}(t)V_{\mathscr{H}}(s)\phi\|^2 \leqslant C^2\|\phi\|^2$,

(iii) $E\|V_{\mathscr{H}}(t)V_{\mathscr{H}}(s)\phi\|^2 \leqslant C^2\|\phi\|^2$,

(iv) $E\left\|\int_s^t dq\, V_{\mathscr{H}}(q)\phi\right\|^2 \leqslant C^2(t-s)\|\phi\|^2$.

Proof: We now prove part (i).

Let $\phi\in\mathscr{H}$ and $t\geqslant 0$, we have

$$E\|V_{\mathscr{H}}(t)\phi\|^2 = E\left(\sum_{n\in\mathbb{Z}^3} v_n(t)P_n\phi, \sum_{m\in\mathbb{Z}^3} v_m(t)P_m\phi\right)$$

$$= E\sum_{n\in\mathbb{Z}^3} v_n(t)^2\|P_n\phi\|^2 = g_0\|\phi\|^2.$$

We skip the proof of parts (ii)–(iv), since it follows from calculus analogous to the one used above. $\square$

The next lemma gives the infinitesimal generator of the limit semigroup. This refers to condition (D) of Sec. 2 (in Ref. 2).

Lemma 3.3: There exists in $\mathscr{H}$, for each $\phi\in\mathscr{H}$, the strong limit

$$s-\lim_{t\to\infty} \frac{1}{t}\int_0^t ds \int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}.$$

Proof: Let $\phi\in\mathscr{H}$ and $0\leqslant r\leqslant s$. We have

$$E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}$$

$$= -\sum_{n,m\in\mathbb{Z}^3} g_{n-m}e^{-c(s-r)^2}U_0(-s)P_n U_0(s-r)P_m U_0(r)\phi.$$

Therefore for each $\phi\in B$, we have

$$E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)$$
$$= -e^{-c(s-r)^2}\int_B d\theta_1\int_B d\theta_2\, e^{-is\theta^2}$$
$$\times e^{i(s-r)\theta_1^2}e^{ir\theta_2^2}\phi(\theta_2)\frac{1}{(2\pi)^3}$$
$$\times\sum_{n,m\in\mathbb{Z}^3} g_{n-m}e^{in(\theta-\theta_1)}e^{im(\theta_1-\theta_2)}.$$

Recall that

$$\frac{1}{(2\pi)^{3/2}}\sum_{n\in\mathbb{Z}^3}e^{in\theta}=\delta(\theta).$$

We conclude, using (2.4), that

$$E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)$$
$$=e^{-c(s-r)^2}\int_B d\theta_1\, e^{-i(s-r)(\theta^2-\theta_1^2)}g(\theta-\theta_1)\phi(\theta).$$

Thus, for every $t>0$,

$$\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)$$
$$=\left[-\frac{1}{t}\int_0^t ds\int_0^s dr\, e^{-c(s-r)^2}\right.$$
$$\left.\times\int_B d\theta_1\, e^{-i(s-r)(\theta^2-\theta_1^2)}g(\theta-\theta_1)\right]\phi(\theta).$$

Consequently, for all $\theta\in B$,

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)$$
$$=\left[-\int_0^\infty ds\, e^{-cs^2}\int_B d\theta_1\, e^{-is(\theta^2-\theta_1^2)}g(\theta-\theta_1)\right]\phi(\theta).$$

Using (2.4), for every $t>0$ we obtain

$$\left|\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)\right|$$
$$\leqslant(2\pi)^{3/2}\|g\|_1\int_0^\infty dr\, e^{-cr^2}|\phi(\theta)|.$$

Thus, by the Lebesgue dominated convergence theorem, for every $\phi\in\mathscr{H}$ there exists the strong limit

$$s-\lim_{t\to\infty}\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}$$

in $\mathscr{H}$. □

Definition 3.1: For each $c\geqslant 0$, let $\bar{V}:\mathscr{H}\to\mathscr{H}$ be the operator given by

$$(\bar{V}_c\phi)(\theta)$$
$$=\left[-\int_0^\infty ds\, e^{-cs^2}\int_B d\theta_1\, e^{-is(\theta^2-\theta_1^2)}g(\theta-\theta_1)\right]\phi(\theta)$$
$$=\left[\frac{-\sqrt{\pi}}{2\sqrt{c}}\int_B d\theta_1\, g(\theta-\theta_1)e^{-9(\theta^2-\theta_1^2)/8c}\right]\phi(\theta),$$

for every $\phi\in\mathscr{H}$.

Lemma 3.4: For each fixed $c>0$, $\bar{V}_c$ satisfies the following conditions:

(i) $\bar{V}_c$ is bounded,

(ii) the semigroup $\{S_c(\tau)=\exp(\tau\bar{V}_c):\tau\geqslant 0\}$ is contractive,

(iii) there exists a constant A such that for every fixed $t>0$ and $\phi\in\mathscr{H}$,

$$\left\|\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}-\bar{V}_c\phi\right\|\leqslant\frac{A}{t}\|\phi\|.$$

Proof: Parts (i) and (ii) are trivial and their proofs are omitted.

Take a fixed $\theta\in B$,

$$(\bar{V}_c\phi)(\theta)-\frac{1}{t}\int_0^t ds\int_0^s dr\, E\{V_{\mathscr{H}}(s)V_{\mathscr{H}}(r)\phi\}(\theta)$$
$$=-\int_0^\infty dq\, e^{-cq^2}\int_B d\theta_1\, e^{-iq(\theta^2-\theta_1^2)}g(\theta-\theta_1)\Big\} \tag{3.1}$$
$$+\frac{1}{t}\int_0^t ds\int_0^s dr\, e^{-c(s-r)^2}\int_B d\theta_1$$
$$\times\{e^{-i(s-r)(\theta^2-\theta_1^2)}g(\theta-\theta_1)\phi(\theta).$$

We note that

$$\int_0^\infty dq\, e^{-cq^2}\int_B d\theta_1\, e^{-iq(\theta^2-\theta_1^2)}g(\theta-\theta_1)$$
$$=\frac{1}{t}\int_0^t ds\int_0^s dr\, e^{-c(s-r)^2}\int_B d\theta_1\, e^{-i(s-r)(\theta^2-\theta_1^2)}g(\theta-\theta_1)$$
$$+\frac{1}{t}\int_0^t ds\int_s^\infty dr\, e^{-cr^2}\int_B d\theta_1\, e^{-ir(\theta^2-\theta_1^2)}g(\theta-\theta_1).$$

We now substitute the above expression into Eq. (3.1) and then we majorize the term which is left. We obtain

$$\left|\frac{1}{t}\int_0^t ds\int_s^\infty dr\, e^{-cr^2}\int_B d\theta_1\, e^{-ir(\theta^2-\theta_1^2)}g(\theta-\theta_1)\right|$$
$$\leqslant(2\pi)^{3/2}\|g\|_1\frac{1}{t}\int_0^t ds\int_s^\infty dr\, e^{-cr^2}$$
$$\leqslant\frac{(2\pi)^{3/2}}{2c}\|g\|_1\frac{1}{t}.$$

This concludes the proof of the lemma. □

In order to show that the mixing condition imposed by the limit theorem in Ref. 2 is valid for our system, we need to mention a result found in Ref. 5.

Let $\{f\}$ and $\{f'\}$ be two sets of real-valued random variables belonging to the same Gaussian system. Let $\mathfrak{M}$ and $\mathfrak{M}'$ be the σ-algebras generated, respectively, by the events $\{f\in B\}$ and $\{f'\in B'\}$, where B and B' are arbitrary Borel sets on $\mathbb{R}$. Let $\mathfrak{h}$ and $\mathfrak{h}'$ be the closure in mean square of the linear span, respectively, of $\{f\}$ and $\{f'\}$.

We now introduce a mixing coefficient relating the σ-algebras $\mathfrak{M}$ and $\mathfrak{M}'$.

Definition 3.2: We define

$$\beta(\mathfrak{M},\mathfrak{M}')\equiv\sup\left\{\frac{|E\{(g-Eg)(g'-Eg')\}|}{E^{1/2}|g-Eg|^2E^{1/2}|g'-Eg'|^2}:\ g\in\mathfrak{h}\atop g'\in\mathfrak{h}'\right\}.$$

We call

$$\alpha(\mathfrak{M},\mathfrak{M}')=\sup_{A\in\mathfrak{M},A'\in\mathfrak{M}'}|P(A\cap A')-P(A)P(A')|$$

the maximal correlation coefficient between the σ-algebras $\mathfrak{M}$ and $\mathfrak{M}'$. In Ref. 2, it is proved that under the above assumptions

$$\alpha(\mathfrak{M},\mathfrak{M}') = \beta(\mathfrak{M},\mathfrak{M}'). \tag{3.2}$$

We now define the σ-algebras $\mathscr{A}_s^t$, $0\leqslant s\leqslant t\leqslant\infty$, and the strong mixing coefficient of these σ-algebras used by the limit theorem established in Ref. 2.

Definition 3.3: For every $0\leqslant s\leqslant t\leqslant\infty$, let $\mathscr{A}_s^t$ be the σ-algebra generated by all cylinder sets

$$Z(n_1,\ldots,n_k;r,R) = \{\omega\in\Omega:(v_{n_1}(r),\ldots,v_{n_K}(r))\in R\},$$

where $k\in\mathbb{N}_+$, $n_1,\ldots,n_k\in\mathbb{Z}^3$, $s\leqslant r\leqslant t$ (in case $t=\infty$, $s\leqslant r<\infty$), and $R\in$ B $(\mathbb{R}^k)$. Here B $(\mathbb{R}^k)$ stands for the σ-algebra of Borel sets in $\mathbb{R}^k$.

Definition 3.4: We call α the strong mixing coefficient of the σ-algebras $\mathscr{A}_s^t$, $0\leqslant s\leqslant t\leqslant\infty$, given by the relation

$$\tau\in(0,\infty)\mapsto\sup_{t\geqslant 0}\alpha(\mathscr{A}_0^t,\mathscr{A}_{t+\tau}^{\infty}).$$

The next lemma is linked to condition (A) of Sec. 1 (in Ref. 2).

Lemma 3.5: Let α be the coefficient established by Definition 3.4, then for every $\tau\geqslant 0$,

$$\alpha(\tau) = e^{-c\tau^2}.$$

The proof of this lemma is done in Sec. IV. Let $M^{(\lambda)}(t,s)$, for fixed $0\leqslant s\leqslant t$, be the propagator (or solution) operator of Eq. (2.1). The next result states that Eq. (2.1) is a strong mixing random differential equation.

Lemma 3.6: For every $\phi\in\mathscr{H}$ and $0\leqslant s\leqslant r\leqslant t$, $V_{\mathscr{H}}(r)\phi$ and $M^{(\lambda)}(t,s)\phi$ are weakly $\mathscr{A}_s^t$-*measurable.*

Proof: We only need to show that, for every $\psi\in\mathscr{H}$, the function

$$\omega\in\Omega\mapsto(V_{\mathscr{H}}(r,\omega)\phi,\psi)$$

is $\mathscr{A}_s^t$-measurable.

We rewrite $(V_{\mathscr{H}}(r,\omega)\phi,\psi)$ as

$$\sum_{n\in\mathbb{Z}^3} v_n(r,\omega)(U_{\mathscr{H}}(-r)P_n U_{\mathscr{H}}(r)\phi,\psi)$$

which is a linear combination of $\mathscr{A}_s^t$-measurable functions.

Therefore $V_{\mathscr{H}}(r)\phi$ is weakly $\mathscr{A}_s^t$-measurable. □

The notions of strong and weak measurability are equivalent in a separable space (see Ref. 6).

From trivial considerations on the solution of Eq. (2.1) formulated in Ref. 2, we conclude that, for fixed $0\leqslant s\leqslant t$, $M^{(\lambda)}(t,s)$ is a unitary operator [condition (C) of Sec. 2 in Ref. 2].

We thus obtain by the limit theorem proved in Ref. 2:

Theorem 3.1: For each fixed $\tau\geqslant 0$ and $\phi\in\mathscr{H}$, in the weak sense

$$\omega-\lim_{\lambda\to 0+} E\{M^{(\lambda)}(\tau/\lambda^2,0)\phi\} = S_c(\tau)\phi.$$

We have noticed that so far our analysis holds for a model consisting of any lattice $\mathbb{Z}^d$, where $d\in\mathbb{N}$. The method developed by Martin and Emch is carried out only for $d\geqslant 3$.

IV. THE STATIONARY GAUSSIAN PROCESS $\{v_n(t)\}$

We will sketch here the construction of a probability space $(\Omega,\mathscr{A},P)$ and will define in this space a stationary Gaussian process which satisfies condition (2.3). We will follow the analysis developed by Hida in Ref. 7 which employs the notion of nuclear space together with the so-called Bochner–Minlos theorem. In order to state this result we consider E to be the nuclear space $\mathscr{S}(\mathbb{R}^4)$ of all real-valued rapidly decreasing functions defined on $\mathbb{R}^4$ and its dual $E^* = \mathscr{S}'(\mathbb{R}^4)$.[8,9] We recall that E^* is also a nuclear space.[10]

We conclude this section showing that the operator V (defined in Lemma 3.1) is unbounded and proving Lemma 3.5.

We say that $C:\xi\in E\mapsto C(\xi)\in\mathbb{C}$ is a characteristic functional on E (Ref. 7), if

(i) C is continuous on E,
(ii) C is positive-definite, and
(iii) $C(0)=1$.

The Bochner–Minlos theorem states that, given a characteristic functional C on E, there exists a unique probability measure P on the pair $(E^*,\mathscr{A})$, where $\mathscr{A}$ is the σ-algebra generated by all cylinder sets in E^* (see Ref. 7, p. 65), which satisfies the equation

$$C(\xi) = \int_{E^*}\exp(i\langle\omega,\xi\rangle)P(d\omega).$$

Thus, in order to construct a generalized Gaussian process (E^*,P) as defined in Ref. 7, it is necessary that the random variable $\omega\mapsto\langle\omega,\xi\rangle$ has a characteristic functional of the form:

$$C(\xi) = \exp(m(\xi) - \tfrac{1}{2}k(\xi,\xi)),$$

where $m(\xi)$ and $K(\xi,\xi)$ are, respectively, its mean and variance. The stochastic process $\{v_n(t)\}$ satisfies condition (2.3). With this in mind, we now define a suitable characteristic functional C.

Let $\{\xi_n\in\mathscr{S}(\mathbb{R}^3):n\in\mathbb{Z}^3\}$ be an orthonormal basis in the Hilbert space $\mathfrak{X} = \mathscr{L}^2(\mathbb{R}^3)$, with norm $\|\cdot\|_2$ and inner product $(\cdot,\cdot)_2$. Furthermore, we assume that ξ_n are real-valued functions.

We call G the bounded self-adjoint operator acting in $\mathfrak{X}$ defined by the relation

$$\xi_n\mapsto\sum_{m\in\mathbb{Z}^3} g_{n-m}\xi_m. \tag{4.1}$$

From (2.4) it follows that $g(\theta)$ is a continuous positive function on the compact set B, thus there exist the square root operators $G^{1/2}$ and $G^{-1/2}$.

Therefore, we can use G to define a new inner product. We call $(\cdot,\cdot)_G$ the inner product defined by

$$(\xi,\eta)_G = (G\xi,\eta)_2,$$

for every $\xi,\eta\in\mathfrak{X}$. Let $\mathfrak{X}_G$ be the Hilbert space given by the completion of the linear space $\mathfrak{X}$ with respect to the inner product $(\cdot,\cdot)_G$.

Let $\|\cdot\|_0$ be the norm in the Hilbert space $\mathfrak{h} = \mathscr{L}^2(\mathbb{R}^4)$. We note that if $f\in\mathfrak{h}$,

$$f:(s,x)\in\mathbb{R}\times\mathbb{R}^3\mapsto f(s,x)\in\mathbb{C},$$

then the function

$$f_s:x\in\mathbb{R}^3\mapsto f(s,x)$$

belongs to $\mathfrak{X}$ for almost all $s\in\mathbb{R}$.

Let $(\cdot,\cdot)_\Gamma$ be the inner product given by

$$(f^{(1)},f^{(2)})_\Gamma = \int_{-\infty}^{\infty} ds (f_s^{(1)},f_2^{(2)})_G,$$

for every $f^{(1)},f^{(2)}\in\mathfrak{h}$. We call $\mathfrak{h}_\Gamma$ the Hilbert space defined by the completion of the linear space $\mathfrak{h}$ with respect to the inner product $(\cdot,\cdot)_\Gamma$. Let $\|\cdot\|_\Gamma$ be the norm in the space $\mathfrak{h}_\Gamma$.

Our characteristic functional is then

$$C:\gamma\in E\mapsto \exp(-\|\gamma\|_\Gamma^2/2).$$

By the Bochner–Minlos theorem this defines uniquely a probability measure P on $(E^*,\mathscr{A})$ such that

$$C(\gamma) = \int_{E^*} \exp(i\langle\omega,\gamma\rangle) P(d\omega),$$

for every $\gamma\in E$.

Set $\Omega = E^*$. We now construct a stochastic process, namely $v_n(t)$, defined in $(\Omega,\mathscr{A},P)$ which satisfies condition (2.3).

We recall that through this section, c is a fixed positive constant.

We define

$$h_c:s\in\mathbb{R}\mapsto[(2c)^{1/4}/\sqrt{\pi}]\exp(-2cs^2)\in\mathbb{R}.$$

For every $n\in\mathbb{Z}^3$, we set

$$\gamma_n:(s,x)\in\mathbb{R}\times\mathbb{R}^3\mapsto h_c(s)\xi_n(x)\in\mathbb{R}.$$

Because $\xi_n\in\mathscr{S}(\mathbb{R}^3)$ and $h_c\in\mathscr{S}(\mathbb{R})$, $\gamma_n\in E=\mathscr{S}(\mathbb{R}^4)$.

Finally, we define the real-valued random variables v_n, for $n\in\mathbb{Z}^3$, by

$$\omega\in\Omega\mapsto\langle\omega,\gamma_n\rangle.$$

For fixed $t\in\mathbb{R}$, we call $S(t)$ the shift transformation given by

$$\gamma(\cdot,\cdot,\cdot,\cdot)\in E\mapsto\gamma(\cdot-t,\cdot,\cdot,\cdot)\in E.$$

Thus $\{S(t):t\in\mathbb{R}\}$ is a one-parameter group of transformations acting on E. This defines on $(\Omega,\mathscr{A},P)$ a group of measure-preserving transformations $\{T(t);t\in\mathbb{R}\}$ acting on Ω as follows:

$$\langle T(t)[\omega],\gamma\rangle = \langle\omega,S(t)\gamma\rangle,$$

for every $\omega\in\Omega$ and $\gamma\in E$.

To each fixed $n\in\mathbb{Z}^3$, we define the stochastic process

$$v_n(t):\omega\in\Omega\mapsto\langle T(t)[\omega],\gamma_n\rangle,$$

for every $t\geqslant 0$.

Clearly, we have for every $\gamma,\zeta\in E$ that

(i) $E\{\langle\cdot,\gamma\rangle\}=0$,

(ii) $E\{\langle\cdot,\gamma\rangle\langle\cdot,\zeta\rangle\}=(\gamma,\zeta)_\Gamma$.

It implies that $\{v_n(t)\}$ is a Gaussian stationary process which satisfies condition (2.3).

We now prove that the interaction potential at $t=0$,

$$V=\sum_{n\in\mathbb{Z}^3} v_n P_n,$$

is indeed an unbounded operator. For this we use the following corollary of the Borel–Cantelli lemma (see Ref. 11).

Corollary: Let $\{X_k:k\in\mathbb{Z}^+\}$ be an independent Gaussian chain obeying the law $\mathfrak{N}(0,1)$ in the probability space $(\Omega,\mathscr{A},P)$, i.e., $E\{X_k\}=0$ and $E\{|X_k|^2\}=1$. Then we have that

$$P\{\omega:\textit{the sequence } X_k(\omega) \text{ is unbounded}\}=1.$$

Theorem 4.1: There exists $\Omega_0\in\mathscr{A}$, with $P(\Omega_0)=1$, such that for every $\omega\in\Omega_0$

$$V(\omega)=\sum_{n\in\mathbb{Z}^3}\langle\omega,\gamma_n\rangle P_n$$

is an unbounded operator acting in $\mathscr{H}$.

Proof: It is sufficient to prove that

$$P\{\omega\in\Omega:\text{the chain }\langle\omega,\gamma_n\rangle \text{ is unbounded}\}=1.$$

Recall that for each $n\in\mathbb{Z}^3$

$$\gamma_n = h_c\xi_n\in E,$$

where $\{\xi_n:n\in\mathbb{Z}^3\}$ is a basis in the space $\mathfrak{X}_G$.

Using the Gram–Schmidt orthogonalization theorem, we obtain an orthonormal basis $\{e_m:m\in\mathbb{Z}^3\}$ in $\mathfrak{X}_G$. Thus $\{Y_m=\langle\cdot,e_m\rangle:m\in\mathbb{Z}\rangle$ is an independent Gaussian chain with the law $\mathfrak{N}(0,1)$.

Because ξ_n, $n\in\mathbb{Z}^3$, can be written as a finite linear combination of e_n, $n\in\mathbb{Z}^3$, the conclusion of the theorem follows from the above corollary. □

In order to prove Lemma 3.5, where we define the strong mixing coefficient of our system, we need some definitions.

Clearly, the vectors $\eta_n = G^{-1/2}\xi_n, n\in\mathbb{Z}^3$, form an orthonormal basis in $\mathfrak{X}_G$. Using the Fourier transform, we obtain that

$$\eta_n=\sum_{m\in\mathbb{Z}^3} c_{n-m}\xi_m,$$

where for each $n\in\mathbb{Z}^3$

$$c_n=\frac{1}{(2\pi)^{3/2}}\int_B d\theta\, e^{-in\theta}\frac{1}{(g(\theta))^{1/2}}.$$

We now prove Lemma 3.5.

For convenience we work with the random variables

$$z_n(t)=\sum_{m\in\mathbb{Z}^3} c_{n-m}v_m(t),$$

$n\in\mathbb{Z}^3$, $t\geqslant 0$, instead of $v_n(t)$, since both sets, $\{v_n(t)\}$ and $\{z_n(t)\}$, generate the same σ-algebras $\mathscr{A}_s^t$, $0\leqslant s\leqslant t\leqslant\infty$.

Recall that $\mathscr{F}=\mathscr{L}^2(\Omega,\mathscr{A},P)$. For $0\leqslant s\leqslant t\leqslant\infty$, let

$$F_s^t=\left\{\sum_{n\in\mathbb{Z}^3} a_n z_n(r_n)\in\mathscr{F}:a_m\in\mathbb{R},\quad s\leqslant r_m\leqslant t,\quad \forall m\in\mathbb{Z}^3\right\}.$$

If $z=\sum_{n\in\mathbb{Z}^3} a_n z_n(r_n)\in F_s^t$, then

$$E\{z^2\}=\sum_{n\in\mathbb{Z}^3} a_n^2<\infty.$$

Let $t>0$ and $\tau\leqslant 0$ and take

$$x=\sum_{n\in\mathbb{Z}^3} a_n z_n(r_n)\in F_0^t$$

and

$$y=\sum_{m\in\mathbb{Z}^3} b_m z_n(s_n)\in\bigcup_{r>t+\tau} F_{t+\tau}^r$$

such that $E\{x^2\}=E\{y^2\}=1$. Consequently, we have that

$$|E\{xy\}=|\sum_{n\in\mathbb{Z}^3} a_n b_n e^{-c(s_n-r_n)^2}|$$

$$\leqslant \sum_{n\in\mathbb{Z}^3} |a_n b_n| e^{-c\tau^2}$$

$$\leqslant e^{-c\tau^2},$$

since $s_n - r_n \geqslant \tau$, for all $n\in\mathbb{Z}^3$.

However, if for a fixed $n\in\mathbb{Z}^3$, we define $x = z_n(t)$ and $y = z_n(t+\tau)$,

$$E\{xy\} = e^{-c\tau^2}.$$

Then by Definition 3.2,

$$\beta(\mathscr{A}_0^t, \quad \mathscr{A}_{t+\tau}^{\infty}) = e^{-c\tau^2}.$$

Thus from (3.2) and Definition 3.4 follows that

$$\alpha(\tau) = e^{-c\tau^2}. \qquad \square$$

V. CONCLUSIONS

In Ref. 2, an analysis was developed to study the asymptotic limit of time-evolutions in Hilbert space through the use of random differential equations of the form (2.1). This analysis is a variation of the method presented by Cogburn and Hersh[12] and Papanicolaou and Varadhan.[13] One of the differences between the results proved in Ref. 2 and Refs. 12 and 13 is that the result in the latter permits the random framework of the abstract model to be described by a Gaussian system (see Ref. 14).

With respect to the study of the validity of the van Hove's long-time, weak-coupling limit we have achieved some improvements. One is that we were able to construct a model for which the existence of this limit is not restricted to a finite radius of convergence. Another one is that the dispersion law $\theta \mapsto \theta^2$ can be modified and the proof does not collapse. In particular, we can consider a phonon-type dispersion law which behaves as

$$\theta \mapsto c|\theta|$$

for small θ's, where c is a positive constant.

We also would like to point out that the result obtained for the so called Martin–Emch model can be recovered asymptotically from our assembly of models. We recall that, in our analysis, for each parameter $c > 0$, we have associated a quantum system. The so-called van Hove's limit of each system dynamics is described by the semigroup

$$S_c(\tau) = \exp(\tau \bar{V}_c), \quad \tau \geqslant 0.$$

Consequently, if we show that as $c \to 0^+$, the semigroups $S_c(\tau)$ converge to a semigroup, namely $S_0(\tau)$, which agrees with the one obtained by Martin and Emch, it means that when the new degree of freedom we have introduced is omitted, we recover the original Martin–Emch model. Therefore we have proved that the weak-coupling limit of the dynamics of the Martin–Emch model holds for all rescaled time.

The result that we need to establish in order to carry on this program is as follows.

Theorem 5.1: For each fixed $\tau \geqslant 0$

$$\mathrm{s}-\lim_{c\to 0^+} S_c(\tau) = S_0(\tau).$$

The semigroup $\{S_0(\tau) = \exp(\tau \bar{V}_0) : \tau \geqslant 0\}$ is the van Hove's limit obtained by Martin and Emch in Ref. 3.

The proof of Theorem 5.1 follows directly from the next lemma.

Lemma 5.1: For every $\theta\in B$, the path

$$\alpha_\theta : c\in[0,\infty) \mapsto \int_0^\infty ds\, e^{-cs^2} \times \int_B d\theta_1\, e^{-is(\theta^2 - \theta_1^2)} g(\theta - \theta_1) \in \mathbb{C}$$

is continuous at $c = 0$, uniformly on θ.

Proof: Let $s > 0$ and $\theta\in B$. By using a simple expansion, we obtain

$$\int_B d\theta_1\, e^{i\theta_1^2 s} g(\theta - \theta_1) = \frac{1}{(2\pi)^{3/2}} \sum_{n\in\mathbb{Z}^3} g_n e^{-in\theta} \times \int_B d\theta_1\, e^{i(s\theta_1^2 + n\theta_1)}.$$

Recalling that

$$\int_{-\infty}^{\infty} \cos x^2 dx = \int_{-\infty}^{\infty} \sin x^2\, dx = \frac{\sqrt{\pi}}{2},$$

after a convenient change of variable, one obtains a constant A, which does not depend on θ, such that

$$\left| \int_B d\theta_1\, e^{i(s\theta_1^2 + n\theta_1)} g(\theta - \theta_1) \right| \leqslant \frac{1}{s^{3/2}} \frac{A}{(2\pi)^{3/2}} \|g\|_1,$$

for every $n\in\mathbb{Z}^3$.

We now show that α_θ is continuous at $c = 0$. Take $0 < \epsilon < 1$. There exists $x_0 > 0$ such that

$$|1 - e^{-x}| \leqslant \epsilon^2,$$

for every $0 \leqslant x \leqslant x_0$.

Let $0 < c \leqslant x_0 \epsilon^2$. Then

$$\begin{aligned} |\alpha_\theta(0) - \alpha_\theta(c)| &\leqslant \int_0^{1/\epsilon} ds(1 - e^{-cs^2}) \int_B d\theta_1 |g(\theta - \theta_1)| \\ &\quad + \int_{1/\epsilon}^{\infty} ds(1 - e^{-cs^2}) \left| \int_B d\theta_1\, e^{-is(\theta^2 - \theta_1^2)} g(\theta - \theta_1) \right| \\ &\leqslant (2\pi)^{3/2} \|g\|_1 \frac{1}{\epsilon} \epsilon^2 + \frac{A}{(2\pi)^{3/2}} \|g\|_1 \int_{1/\epsilon}^{\infty} ds \frac{1}{s^{3/2}} \qquad (5.1) \\ &\leqslant B\sqrt{\epsilon}, \end{aligned}$$

where the constant B holds for any choice of θ.

We thus conclude that α_θ is continuous at $c = 0$, uniformly on θ. $\square$

From the contractiveness of the semigroup $S_c(\tau)$, $c \geqslant 0$, which is easily seen, and Lemma 5.1 follows the validity of Theorem 5.1.

We point out that, although we can carry on our analysis in any lattice $\mathbb{Z}^d$, we can only derive the asymptotical limit $c \to 0^+$ for $d \geqslant 3$. This is easily observed in the proof of Lemma 5.1, there we need the integrability of the function $s \to s^{-d/2}$ [see (5.1)].

ACKNOWLEDGMENTS

The research described in this paper was done at the Department of Mathematics, University of Rochester,

Rochester, NY. We are happy to thank Professor G. G. Emch for his valuable advice. We are also indebted to Professor H. Spohn for his valuable suggestions.

This work was partially supported by CNPq, Grant 301456/80.

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Triangular Ising model: Complete expressions for even spin correlations in an exact evaluation of $P(h,T)$

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(Received 30 November 1983; accepted for publication 4 May 1984)

Complete expressions of all even correlations for the triangular Ising model in a recent exact evaluation of $P(h,T)$, the local magnetic field distribution, are obtained from the Pfaffian representation derived by Stephenson. The results for the ferromagnetic $J<0$ and antiferromagnetic $J>0$ cases contain a number of interesting features previously not pointed out in the Ising literature. As a bonus, some new inequalities relating odd and even correlations are also obtained.

PACS numbers: 75.10.Hk

I. INTRODUCTION

In a recent series of papers,[1-3] some interests have been revived in the study of the local field distribution $P(h,T)$ for a variety of classical spin models. Two important results which emerged indicate that the statistical mechanics of all two spin interaction systems (with random or regular bonds J_{ij} and in a homogeneous field H) can be reformulated from a knowledge of $P(h,T)$ and moreover this knowledge suffices to determine also the inelastic neutron scattering cross section[4] for Ising systems. Furthermore, as previously observed,[5] an exact determination of $P(h,T)$ is indeed possible in the case of the exactly soluble two-dimensional Ising model in a variety of lattices.[6-9] While all these results have been reported,[10] details of the calculations were given only for the square and honeycomb lattices. In these cases all even correlations can be obtained from the literature[11] in terms of elliptic integrals and the three spin correlation is easily related to the spontaneous magnetization[12-16] by an identity of Fisher.[17] The triangular lattice, which has the maximum coordination number of the two-dimensional lattices, of 6, proved to be more complicated. Only Pfaffian expressions were given by Stephenson,[18] who first evaluated the even correlations by generalizing the theory of Montroll, Potts, and Ward.[19] The use of the Pfaffian formulation is strictly not necessary. Presumably similar results can also be derived from spinor algebra, as originally used by Onsager and Kaufman,[20] Yang,[21] and Houtappel,[22] although the analysis is in general more complicated. The purpose of this paper is to provide explicit (and therefore computable) expressions for all even correlations hitherto unpublished in the exact evaluation of $P(h,T)$ (see Ref. 23). In Sec. II we obtain explicit expressions for all even correlations in terms of 11 integrals which can all be reduced to expressions containing complete elliptic integrals.

In Sec. III we discuss their use in obtaining $P(h,T)$ and in conclusion we examine the physical consequences of these results. As a bonus we obtained a new set of correlation inequalities relating odd and even correlations.

II. EVEN CORRELATIONS

Labeling the center spin as σ_0 and its six nearest neighbors cyclically from σ_1 to σ_6 on the isotropic triangular lattice, we require evaluation of the following even correlations for the purpose of obtaining $P(h,T)$:

$$\begin{aligned} &S_{01}=S_{12}=\langle\sigma_0\sigma_1\rangle, \quad S_{13}=\langle\sigma_1\sigma_3\rangle,\\ &S_{14}=\langle\sigma_1\sigma_4\rangle, \quad S_{1245}=\langle\sigma_1\sigma_2\sigma_4\sigma_5\rangle,\\ &S_{1234}=\langle\sigma_1\sigma_2\sigma_3\sigma_4\rangle, \quad S_{1235}=\langle\sigma_1\sigma_2\sigma_3\sigma_5\rangle,\\ &S_6=\langle\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\rangle. \end{aligned} \tag{1}$$

The details for obtaining these correlations by considering perturbed dimer configurations are given by Stephenson,[24] in the form of Pfaffians. In this section we shall use his notation for the Pfaffian elements, of which there are 31 for our required correlations. Each element denoted by $(m,n)_{ij}$ is given in the form of the twofold integral

$$(m,n)_{ij}=\frac{(1-v)}{(2\pi)^2}\int_{-\pi}^{\pi}d\phi_1\int_{-\pi}^{\pi}d\phi_2\, e^{-i(m\phi_1+n\phi_2)} \times C_{ji}(\phi_1,\phi_2)/\Delta(\phi_1,\phi_2), \tag{2}$$

where $v=\tanh K$, $K=\beta J$, and the C_{ij} are the cofactor elements of which there are 36. The procedure for obtaining these cofactors is given in the Appendix to Ref. 18. The quantity $\Delta(\phi_1,\phi_2)$ determines the partition function and for the isotropic lattice is given by

$$\begin{aligned} &\Delta(\phi_1,\phi_2)=A+B\cos\phi_2+C\sin\phi_2,\\ &A=(1-2v+6v^2-2v^3+v^4)-2v(1-v)^2\cos\phi_1,\\ &B=-2v(1-v)^2(1+\cos\phi_1),\\ &C=2v(1-v)^2\sin\phi_1. \end{aligned} \tag{3}$$

Not all 31 Pfaffian elements are independent, however. By exploiting the symmetry of the twofold integrals (1) under the transformations $\phi_1\to\omega+\theta,\phi_2\to-\theta$, as well as $\Delta(\phi_1,\phi_2)=\Delta(\phi_2,\phi_1)$, the number of independent elements reduces to 19. One further reduction in the number of integrals to be evaluated can be further achieved. This is by avoiding a direct evaluation of S_{1235} which, like S_6, is given in terms of a (6×6) Pfaffian containing 15 terms in its expansion. In this way, the number of integrals to be evaluated reduces to 11, thereby obtaining a considerable saving in labor. We finally obtain σ_{1235} from all the rest by using Fisher's identity,[25] although Stephenson originally used it as a consistency check. Expansion of the Pfaffian expressions for the various correlations gives

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$$S_{01} = S_{12} = v + (1,1)_{ST}, \tag{4}$$

$$S_{13} = S_{12}^2 - (1,0)_{RS}^2 - (2,1)_{RT}(0,0)_{LS}, \tag{5}$$

$$S_{14} = S_{12}^2 + (2,2)_{RT}(0,0)_{TS}, \tag{6}$$

$$S_{1245} = S_{12}^2 + (-1,1)_{SS}^2 - (0,2)_{ST}^2, \tag{7}$$

$$S_{1234} = S_{12}^2 + (-2,0)_{US}(1,1)_{LU} - (-2,-1)_{DS}^2, \tag{8}$$

$$\begin{aligned} S_6 = {} & S_{12}S_{1234} - 2(-2,-1)_{DS}^2[S_{12} + (1,1)_{LU} - (-2,0)_{US}] \\ & + (-2,0)_{US}[(1,1)_{LU}S_{12} + (-2,-1)_{DS}^2 - (-2,0)_{US}^2] \\ & + (1,1)_{LU}[(1,1)_{LU}^2 - (-2,-1)_{DS}^2 + (-2,0)_{US}S_{12}], \end{aligned} \tag{9}$$

and from Fisher's identity

$$\begin{aligned} S_{1235} = {} & \{S_{12} - C(1 + 2S_{12} + 2S_{13} + S_{14}) \\ & - D(4S_{12} + 4S_{13} + 2S_{14} + 4S_{1234} + 2S_{1245}) \\ & - E(2S_{1234} + S_{1245} + S_6)\}\{4D + 2E\}^{-1}, \end{aligned} \tag{10}$$

where

$$\begin{aligned} C &= \tfrac{1}{32}(\tanh 6K + 4\tanh 4K + 5\tanh 2K), \\ D &= \tfrac{1}{32}(\tanh 6K - 3\tanh 2K), \\ E &= \tfrac{1}{32}(\tanh 6K - 4\tanh 4K + 5\tanh 2K). \end{aligned} \tag{11}$$

In the Appendix we list the complete expressions for all 11 Pfaffian elements. One of the integrals in (2) can easily be performed by contour integration. The remaining one as given in the Appendix can be reduced to complete elliptic integrals;[26] for instance,

$$\begin{aligned} (1,1)_{ST} = \frac{2g}{\pi}\Bigg\{\Bigg[\Bigg(\frac{(1+v)^3 - 4v^2}{2(1-v)}\Bigg) + \alpha\Bigg(\frac{5v^2-1}{2v}\Bigg)\Bigg]\mathbb{K}(k') \\ + (1-\alpha)\Bigg(\frac{5v^2-1}{2v}\Bigg)\Pi\Bigg(\frac{2}{\alpha+1}, k'\Bigg)\Bigg\}, \end{aligned} \tag{12}$$

where

$$\begin{aligned} g &= [(\beta-1)(\alpha+1)]^{-1/2}, \quad k'^2 = \frac{2(\beta-\alpha)}{(\beta-1)(\alpha+1)}, \\ \alpha &= (\eta+1) - (3+2\eta)^{1/2}, \quad \eta = \frac{(1+v^2)^3 + 8v^3}{2v(1-v^2)^2}, \\ \beta &= (\eta+1) + (3+2\eta)^{1/2}, \end{aligned} \tag{13}$$

for the ferromagnetic case. The antiferromagnetic case is best obtained by analytic continuation to complex k' from (11).

TABLE I. Critical values for the 11 Pfaffian elements.

Element	Ferromagnetic $T = T_c$	Antiferromagnetic $T = 0$
$(1,1)_{ST}$	$\sqrt{3} - \frac{4}{3}$	$\frac{2}{3}$
$(1,0)_{RS}$	$\frac{2}{3} - \sqrt{3}/\pi$	$-\frac{1}{3} + \sqrt{3}/2\pi$
$(2,1)_{RT}$	$-\frac{2}{3}(1+\sqrt{3}) + (\sqrt{3}/\pi)(\sqrt{3}+2)$	$\frac{1}{3} + \sqrt{3}/2\pi$
$(0,0)_{LS}$	$\frac{2}{3}(1-\sqrt{3}) + (\sqrt{3}/\pi)(\sqrt{3}-2)$	$-(\frac{1}{3} + \sqrt{3}/2\pi)$
$(2,2)_{ST}$	$(\frac{2}{3} - 2/\pi)(2\sqrt{3}+3)$	$-\sqrt{3}/\pi$
$(0,0)_{TS}$	$(\frac{2}{3} + 2/\pi)(2\sqrt{3}-3)$	$\sqrt{3}/\pi$
$(1,-1)_{SS}$	$\frac{16}{3} - 10\sqrt{3}/\pi$	$\sqrt{3}/2\pi - \frac{2}{3}$
$(0,2)_{ST}$	$\frac{20}{3} - 12\sqrt{3}/\pi$	$\frac{2}{3} - 3\sqrt{3}/2\pi$
$(-2,0)_{US}$	$\frac{1}{6}(14\sqrt{3}+13) - (4/\pi)(\sqrt{3}+3)$	$\frac{2}{3} - \sqrt{3}/\pi$
$(1,1)_{LU}$	$\frac{1}{6}(14\sqrt{3}-13) + (4/\pi)(\sqrt{3}-3)$	$-\frac{2}{3} + \sqrt{3}/\pi$
$(-2,1)_{DS}$	$13\sqrt{3}/6 - 12/\pi$	0

The resulting expressions are not unique, however, as may be seen from the addition formulas of elliptic integrals as well as the Landen transformation[27] in the parameter k', here chosen such that $k' \leqslant 1$ for $T \gtrsim T_c$. The formulas for this reduction to complete elliptic integrals like (12) are extremely intricate. For practical purposes it is simplest to evaluate directly the integrals as given in the Appendix by numerical methods. At the ferromagnetic critical point $v = v_c = 2 - \sqrt{3}$ and the antiferromagnetic zero point $v = v_0 = -1$, however, they reduce to elementary integrals that can be evaluated exactly. These values are tabulated in Table I. With these values and Eqs. (3)–(9) we easily obtain exact critical values for our even correlations.[28] Since the number of terms in an $(m \times m)$ Pfaffian expansion grows as $(m-1)!!$ an evaluation of S_6 and S_{1235} by Pfaffians represents perhaps the limit for human computation. For periodically frustrated lattices with a larger repeated cell, or indeed for the eight spin correlation, some form of computer symbolic manipulation becomes essential.

III. $P(h,T)$

Following Ref. 1, the local magnetic field probability distribution for the Ising model

$$H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j, \quad \langle ij\rangle \text{ nearest neighbors} \tag{14}$$

is given by

$$P(h,T) = \Big\langle \delta(h - \sum_j \sigma_j)\Big\rangle, \quad h = H/J, \tag{15}$$

where the sum is over nearest neighbors to σ_i. As noted in Ref. 2, $P(h,T)$ determines all thermodynamic quantities through the magnetization

$$M = N\int dh\, \tanh(\beta h)P(h,T), \quad \beta = 1/k_B T, \tag{16}$$

and internal energy

$$U = -\frac{N}{2}\int dh\, \tanh(\beta h)P(h,T). \tag{17}$$

It further contains information on the neutron scattering cross section:

$$\begin{aligned} S(k,\omega) &= \frac{1}{8\pi}\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\sum_i \langle \sigma_i^+\ \sigma_i^-(t) + \sigma_i^-\ \sigma_i^+(t)\rangle \\ &= (N/2)\{P(\omega/2) + P(-\omega/2)\}/(1 + e^{-\beta\omega}), \end{aligned} \tag{18}$$

where $\sigma^{\pm}$ are the Pauli raising and lowering operators. Thus apart from its simple physical interpretation as a local field distribution, the above exact relations provide a strong motivation for the calculation of $P(h,T)$ which can be obtained exactly for two-dimensional Ising models in a zero field.

Equation (15) is conveniently expanded as

$$\begin{aligned} P(h,T) = {} & \frac{1}{2\pi}\int_{-\infty}^{\infty} d\theta\, e^{-ih\theta}\cos^z\theta \\ & \times \Big\langle \prod_{j=1}^{z}(1 + i\sigma_j\tan\theta)\Big\rangle, \end{aligned} \tag{19}$$

where $z = 6$ for the triangular Ising model and the product is taken round the ring of nearest neighbors to spin σ_0. We easily see that the product in Eq. (19) involves all even correlations given in Sec. II, as well as the odd correlations

$$S_{123} = \langle \sigma_1\sigma_2\sigma_3 \rangle, \quad S_{124} = \langle \sigma_1\sigma_2\sigma_4 \rangle, \quad S_{135} = \langle \sigma_1\sigma_3\sigma_5 \rangle, \tag{20}$$

and

$$S_{12345} = \langle \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5 \rangle,$$

for the ferromagnetic lattice when $T < T_c$ (see Ref. 29).

The simple integrals involved in Eq. (19), can easily be evaluated for the triangular lattice.[30] We shall denote the result in a matrix notation as follows:

$$\mathbf{P} = \hat{M}\mathbf{c}, \tag{21}$$

where

$$\mathbf{c} = \begin{pmatrix} 1 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \\ C_6 \end{pmatrix} = \begin{pmatrix} 1 \\ 6m \\ 6S_{12} + 6S_{13} + 3S_{14} \\ 6S_{123} + 12S_{124} + 2S_{135} \\ 6S_{1234} + 6S_{1235} + 3S_{1245} \\ 6S_{12345} \\ S_6 \end{pmatrix}, \tag{22}$$

$$\hat{M} = \frac{1}{64} \times \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 6 & 4 & 2 & 0 & -2 & -4 & -6 \\ 15 & 5 & -1 & -3 & -1 & 5 & 15 \\ 20 & 0 & -4 & 0 & 4 & 0 & -20 \\ 15 & -5 & -1 & 3 & -1 & -5 & 15 \\ 6 & -4 & 2 & 0 & -2 & 4 & -6 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix} \tag{23}$$

and

$$\mathbf{P} = \begin{pmatrix} P(6) \\ P(4) \\ P(2) \\ P(0) \\ P(-2) \\ P(-4) \\ P(-6) \end{pmatrix} \tag{24}$$

are the values for $P(h,T)$ for $h = 6, 4, 2, 0, -2, -4, -6$, respectively.

In Fig. 1 we plot histograms of $P(h,T)$ for the antiferromagnetic triangular lattice. This is to be compared with the ferromagnetic case given in Ref. 2. These are taken at temperature ranges in which S_6 and S_{14} change sign, see Fig. 6 of Ref. 18. The most notable feature is the variation of the peak at $P(0)$, which alternately sharpens and flattens slightly. This coincides with S_6 changing sign twice (and S_{14} changing sign once), as was noted by Stephenson. It seems to be a manifestation of the effect of frustration destroying the system's attempt to order.

Further, on account of the positivity of $\mathbf{P}$, we can write

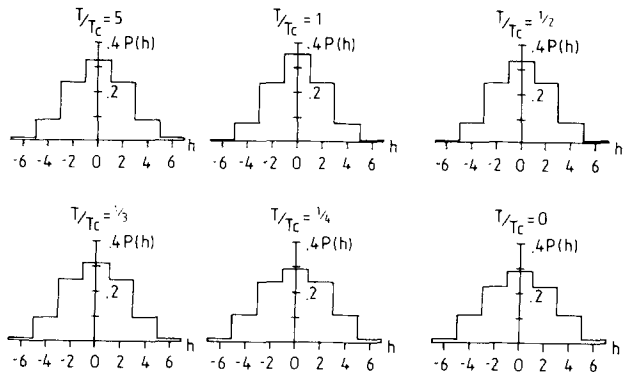

FIG. 1. Histograms of $P(h,T)$ for the isotropic antiferromagnetic triangular Ising model.

down a set of correlation inequalities from (22) relating odd and even correlations; for example

$$15 - C_2 - C_4 + 15S_6 > 0, \quad T > T_c, \tag{25}$$

$$6 - 4C_1 + 2C_2 - 2C_4 + 4C_5 - 6S_6 > 0, \quad T < T_c. \tag{26}$$

However, for reasons given in Ref. 29, our calculations for $T < T_c$ in the ferromagnetic lattice are incomplete.

IV. CONCLUSION

In conclusion, we have evaluated $P(h,T)$ exactly by direct computations of a number of even spin correlations. The main labor comes from the expansion and reduction in the number of Pfaffian elements, which involves evaluation of many integrals. All these expressions are now written in the Appendix. The existence of a dip in the ferromagnetic case[31] for $T > T_c +$ is particularly interesting and seems to have been observed also in computer simulations.[32,33] It appears from these studies that observation of a phase transition from $P(h,T)$ in general is a subtle effect involving the full distribution but for the ferromagnetic case with an infinitesimal field it must be concluded only on the grounds of the onset of asymmetry in the distribution rather than a minimum of $P(h)$ at $h = 0$. It is also interesting to suggest that the features of $P(h,T)$ for the triangular antiferromagnet as indicated above are perhaps universal for a larger class of frustrated or periodically frustrated models that do not order in two dimensions,[34,35] a subject for future study.

ACKNOWLEDGMENTS

I am indebted to Professor David Sherrington for critical reading of this manuscript. Also my special thanks go to Professor John Stephenson and Professor J. H. Barry for valuable discussions during the IUPAP (1983) Statistical Physics conference in Edinburgh.

Financial support of the SERC (U. K.) is gratefully acknowledged.

APPENDIX: COMPLETE EXPRESSIONS FOR THE 11 PFAFFIAN ELEMENTS

$$(1,1)_{ST} = \frac{1}{\pi}\int_0^{\pi} d\theta \frac{(1-v)^2(5v^2-1)\cos\theta + v(1-v)[(1+v)^3 - 4v^2]}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(1,0)_{RS} = \frac{1}{4} + \frac{1}{4\pi}\int_0^\pi d\theta\ \frac{[4v(1-v)^2-\gamma] + [18v(1-v)^2 + 2\gamma - 4(1-v^2)^2]\cos\theta - 4v(1-v)^2\cos^2\theta}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(2,1)_{RT} = -\frac{1}{4v} + \frac{1}{\pi}\int_0^\pi d\theta\ \frac{(\gamma/4v + v^2(1-v)^2) + [2v(1-v^2) - \gamma/2v - (1-v)^2/2]\cos\theta + (1-v)^2\cos^2\theta}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(0,0)_{LS} = \frac{v}{4} + \frac{1}{\pi}\int_0^\pi d\theta\ \frac{[2v(1-v^2) + (v^2/2)(1-v)^2 + v\gamma/2]\cos\theta - ((1-v)^2 + \gamma v/4) - v^2(1-v)^2\cos^2\theta}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(2,2)_{RT} = \frac{v}{2} + \frac{1}{\pi}\int_0^\pi d\theta$$
$$\times\frac{[(1-v^2)(1-v)^2 - \gamma v/2] + [v(1-v)((1+v)^3 - 4v^2) + 3v^2(1-v)^2 + v\gamma]\cos\theta - [2v^2(1-v)^2 + 2(1-v^2)(1-v)^2]\cos^2\theta}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(0,0)_{TS}$$
$$= \frac{-v}{2} + \frac{1}{\pi}\int_0^\pi d\theta\ \frac{[v\gamma/2 + (1-v^2)(1-v)^2] - [v(1-v)((1+v)^3 - 4v^2) + 3v^2(1-v)^2 + v\gamma]\cos\theta + 2v^2(1-v)^2\cos^2\theta}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(1,1)_{LU}$$
$$= -\frac{1}{2} + \frac{1}{\pi}\int_0^\pi d\theta\ \frac{[(1-v^2) - (\gamma + 3v(1-v)^2)]\cos\theta - [2v^2(1-v^2) + 2v(1-v)^2]\cos^2\theta + v^2(1-v^2) + (\gamma/2 + 2v(1-v)^2)}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(-1,1)_{SS} = -\frac{1}{2} - \frac{1}{\pi}\int_0^\pi d\theta\ \frac{\gamma v(1-v)^2\cos^3\theta - 2(\gamma + v(1-v)^2)\cos^2\theta + (\gamma + v(1-v)^2)\cos\theta + \gamma/2}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(0,2)_{ST} = \left(\frac{(1+v)^3 - 4v^2}{4(1-v)}\right) - \frac{v}{2} + \frac{1}{\pi}\int_0^\pi d\theta\ \Bigg\{\Bigg[\left(\eta + \frac{1}{2}\right)(1-v)((1+v)^3 - 4v^2)v + 3v^2(1-v)^2 - \gamma v\Bigg]\cos\theta$$
$$+ [2(\gamma + v(1-v)^2)v - (1-v^2)2(1-v)^2 - v(1-v)((1+v)^3 - 4v^2)]\cos^2\theta - 4v^2(1-v)^2\cos^3\theta$$
$$+ (1-v^2)(1-v)^2 - \frac{\gamma v}{2} - \frac{\eta v}{2}(1-v)((1+v)^3 - 4v^2)\Bigg\}$$
$$\times[\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}]^{-1},$$

$$(-2,0)_{US} = \frac{1}{2} + \frac{1}{\pi}\int_0^\pi d\theta$$
$$\times\frac{[(\gamma + 3v(1-v)^2) + v^2(1-v^2)]\cos\theta + [2v(1-v)^2 - 2(1-v^2)]\cos^2\theta + (1-v^2) - (\gamma/2 + 2v(1-v)^2)}{\{a^2 + (b-c)^2 - 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}},$$

$$(-2,-1)_{DS} = \frac{1-v^2}{4v} + \frac{1}{\pi}\int_0^\pi d\theta\ \{[(1-v)^2(1-v^2)/2](2\eta + 1) - v(1-v^2)\}\cos\theta - [(1-v^2)(1-v)^2$$
$$+ [2v(1-v^2)]\cos^2\theta - \{[(1-v^2)(1-v)^2/2]\eta - v(1-v^2)\}[\{a^2 + (b-c)^2$$
$$- 2a(b+c)\cos\theta + 4bc\cos^2\theta\}^{1/2}]^{-1},$$

where

$$\gamma = [(1+v^2)^3 + 8v^3]/(1+v)^2, \quad \eta = \gamma/2v(1-v)^2,$$

and

$$a = 2v(1+v^2), \qquad b = v^2c, \qquad c = (1-v)^2.$$

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ERRATUM

Erratum: Electrovac type *D* solutions with cosmological constant [J. Math. Phys. 25, 1951 (1984)]

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(Received 9 August 1984; accepted for publication 17 August 1984)

PACS numbers: 04.20.Jb, 99.10. + g

In Table I, the definition of $S(\mu z)$ given in the row $B-R$ should read $S(\mu z)=\nu-\mu z^2$, where $\nu=\{1,0,-1\}$ and μ is a certain constant assuming its real values independently of the values of ν. [In particular, when $\mu=\epsilon=\{-1,0,1\}$ for each choice of ν there are three possibilities for selecting μ. Some of the resulting functions S for a given choice of ν and μ have to be excluded because of the used signature $(+\ +\ +\ -)$.] Thus, in the row $B-R$, the ν used in P runs its values independently of the values assigned to the ν appearing in Q. In the row $gR-N$, the fourth term of Q should be $(e^2+g^2)y^4$. In g^*R-N, the polynomial of the fourth degree in x should be denoted by P. In gC, the function p should be $p=0$, while the polynomial of the fourth degree in x should be denoted by P. In $g\tilde{B}(+)$, the third term of Q should be $+\lambda l^4$. In the row $g\tilde{B}(-)$, the Q should be $Q=S(\epsilon y)$. In the row $P-C[A]$, in ω the external differential operator "d" in front of the parenthesis was omitted. In the row $P-D$, the signs of the second, third, and fourth terms of $Q(y)$ should be reversed.

In the definitions of e^1 and e^2 [Eq. (A3)] the function m should be replaced by p.

In formulas (A5), the imaginary part of $C^{(3)}$ was omitted,

$$\operatorname{Im} 2\Delta H^{-2}C^{(3)}=\frac{p_y}{\Delta}\left[P_x-2\frac{m_x}{\Delta}P\right]+\frac{m_x}{\Delta}\left[Q_y+2\frac{p_y}{\Delta}Q\right].$$

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