

Generating functions for polynomial irreducible tensors

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A general method for constructing a generating function for all irreducible polynomial tensors, with respect to a given compact semisimple group, out of a given set of tensors is derived. The method is applied to the construction of polynomial bases for the IR's of a group reduced according to a subgroup and to the finding of subgroup scalars in the enveloping algebra of a group. A number of examples are worked out.

1. INTRODUCTION

The problem of finding all irreducible tensors, with respect to a compact semisimple group, whose components are polynomials in the components of one or more given tensors is considered. These tensors are described implicitly by a generating function expressed in terms of an integrity basis, i. e., a finite number of "elementary" tensors in terms of which all may be expressed as stretched products. The method is a generalization of that used by Judd, Miller, Patera, and Winternitz¹ to find $O(3)$ invariant polynomials in the generators of $SU(3)$.

The technique is applied to the problem of constructing all such subgroup invariants contained in the enveloping algebra of a semisimple group. It is usually advantageous to divide the group generators first into two sets of subgroup tensors.² Next find all subgroup tensors which are polynomials in the tensors of each set (the problem addressed by this article). Subgroup scalars correspond to contractions of tensors, one from each set, which transform by conjugate subgroup IR's.

A second type of example concerns the construction of polynomial bases of a group. Such bases may be chosen as polynomials in the states of the fundamental IR's; the degrees in the fundamental IR's are the Cartan labels of the IR to which a particular polynomial belongs. When the bases are reduced according to some semisimple subgroup, the states are just subgroup tensors whose components are polynomials in the tensors comprising the fundamental IR's. A complication here is the necessity of eliminating unwanted states, i. e., polynomials belonging to group IR's lower than their degrees would indicate. The members of the resulting integrity basis are the elementary multiplets³ (elementary permissible diagrams of Devi and Moshinsky⁴) which generate all subgroup multiplets belonging to all group IR's and hence solve the corresponding labeling problem.

Section 2 contains a description of the general method with a few simple examples.

In Sec. 3 we derive integrity bases for $O(5)$ polynomial bases reduced according to $SU(2)$.

In Sec. 4 we find an integrity basis for $SU(2)$ scalars in the enveloping algebra of $O(5)$ and for $SU(2) \times SU(2)$ scalars in the enveloping algebra of G_2 ; the latter is shown to be simply related to an integrity basis for

$O(5) \supset SU(2)$ polynomial bases, discussed in Sec. 3. We also consider briefly the integrity basis for $SU(2) \times SU(2)$ scalars in the enveloping algebra of $SU(4)$.

Section 5 contains a discussion of the results and suggestions for further work.

2. GENERATING FUNCTIONS FOR TENSORS

As a simple example, consider the problem of finding all $SU(2)$ tensors whose components are polynomials in the components of a single $\lambda = 3$ ($j = \frac{3}{2}$) tensor U . A generating function for $SU(2)$ weights is

$$[(1 - U\eta^3)(1 - U\eta)(1 - U\eta^{-1})(1 - U\eta^{-3})]^{-1}; \quad (1)$$

the coefficient of $U^a \eta^b$ is the number of terms of degree a in U and weight b (the weight here is, to avoid fractions, twice the conventional m value). The generating function for tensors belonging to the IR λ (highest weight λ , lowest weight $-\lambda$) is the coefficient of $\eta^{-\lambda}$ minus the coefficient of $\eta^{-\lambda-2}$ (the subtraction eliminates the contribution of higher tensors). Formally this difference is found by multiplying by $\eta^{\lambda-1} - \eta^{\lambda+1}$ and summing residues inside the unit η circle ($|U| < 1$ for this purpose).

To keep track simultaneously of tensors belonging to all IR's multiply as well by A^λ and sum over λ from 0 to ∞ . The result is

$$\sum_{\text{res}} (\eta^{-1} - \eta) [(1 - U\eta^3)(1 - U\eta)(1 - U\eta^{-1}) \times (1 - U\eta^{-3})(1 - A\eta)]^{-1}, \quad (2)$$

where \sum_{res} means the sum of residues inside the unit circle ($|A|, |U| < 1$). The result is the generating function

$$G(U, A) = (1 + U^3 A^3) [(1 - UA^3)(1 - U^2 A^2)(1 - U^4)]^{-1}. \quad (3)$$

The coefficient of $U^\alpha A^\lambda$ in G is the number of linearly independent tensors of degree α and IR λ . The generating function (3) may be interpreted in terms of four "elementary" tensors whose degrees and IR's are respectively (1, 3), (2, 2), (4, 0), (3, 3). They constitute an integrity basis for tensors formed from the components of U . Explicit expressions for the elementary tensors as polynomials in the components of U are easily found. That $U^3 A^3$ appears in the numerator of G implies that the (stretched) square of the corresponding tensor is a sum of (stretched) products of the others and hence redundant $[(3, 3)^2 = A(2, 2)^3 + B(1, 3)^2(4, 0)]$. The four tensors are just the elementary multiplets for the IR's $(\lambda, 0)$ of $O(5)$ reduced according to $SU(2)$.³

More generally, consider a generating function $F(\eta_1, \dots, \eta_l)$ for weights with respect to a group G of rank l ; we may assume the weights are those of complete IR's and write

$$F(\eta) = \sum_{\{\lambda\}} \chi_{\lambda_1, \dots, \lambda_l}(\eta) N_\lambda, \quad (4)$$

where χ_λ is the character of the IR λ ; N_λ is essentially the multiplicity of λ in F , and may depend on other dummy variables such as U in Eq. (1).

We recall that the character χ_λ may be expressed in terms of the characteristic ξ_λ by the relation⁵

$$\chi_\lambda = \xi_\lambda / \Delta. \quad (5)$$

Δ is the characteristic of the scalar IR. Thus, Eq. (4) becomes

$$\Delta(\eta)F(\eta) = \sum_{\lambda} \xi_{\lambda_1, \dots, \lambda_l}(\eta) N_\lambda. \quad (6)$$

Let $\Pi_i \eta_i^{M_i}$ be the term of lowest weight in $\xi_\lambda(\eta)$; the M_i depend linearly on $\lambda_1, \dots, \lambda_l$ and we suppose that the coordinates in weight space are chosen so that the coefficients of the λ 's in M_i are all integers. Now multiply Eq. (6) by $\Pi_i \eta_i^{M_i^{-1} A_i}$ and sum over $\lambda_1, \dots, \lambda_l$ from 0 to ∞ . The sums being geometric may be done explicitly. Finally we sum all residues inside the unit circles of η_1, \dots, η_l , regarding A_i , and the dummy variables which carry the degrees of the original tensors, as being less than unity in magnitude.

For definiteness we demonstrate the procedure for $SU(n)$; other semisimple compact groups are treated similarly. We may write⁵

$$\xi_\lambda = |\eta_i^{l-n+j+1}|, \quad \Delta = |\eta_i^{j-1}|, \quad (7)$$

where $|a_{ij}|$ means the $n \times n$ determinant whose ij element is a_{ij} . The l 's are related to the Cartan labels by

$$l_j = \sum_{k=j}^{n-1} \lambda_k + n - j, \quad l_n = 0; \quad (8)$$

also

$$\eta_n = (\eta_1 \eta_2 \cdots \eta_{n-1})^{-1}. \quad (9)$$

We take the term of lowest weight in ξ to be

$$\prod_{i=1}^{n-1} \eta_i^{n-i} (\sum_{k=1}^{n-i} \lambda_k^{n-i}). \quad (10)$$

Thus if $F(\eta_1, \dots, \eta_l)$ is some generating function for $SU(n)$ weights, the corresponding generating function for $SU(n)$ tensors is

$$\sum_{\text{res}} \frac{\Delta(\eta) \prod_{i=1}^{n-2} \eta_i^{n-i-1}}{\prod_{i=1}^{n-1} (1 - A_i \prod_{j=1}^{n-i} \eta_j)} F(\eta_1, \dots, \eta_l). \quad (11)$$

For $n=2$ this reduces to the prescription given above for $SU(2)$.

We list a few simple generating functions for tensors which are polynomials in the components of one or more simple tensors. In each case the integrity basis is easily inferred from the generating function.

(a) $SU(2)$, $\lambda=4$ ($j=2$), tensor U :

$$G(U, A) = (1 + U^3 A^6) / (1 - UA^4)(1 - U^2 A^4)(1 - U^2)(1 - U^3). \quad (12)$$

In a case like this, where only even weights (integer m) are involved, the method may be modified by halving all weights. The effect on the generating function is to replace A^2 by A . With an additional denominator factor $1 - A^2$, Eq. (12) is then the generating function for scalars found from a $j=2$ tensor U and a vector A and agrees with that given in Ref. 1.

(b) $SU(2)$, $\lambda=2$ ($j=1$) vector U and $\lambda=1$ ($j=\frac{1}{2}$), spinor V :

$$G(U, V, A) = (1 + UVA) / (1 - U^2)(1 - UV^2)(1 - UA^2) \times (1 - VA). \quad (13)$$

(c) $SU(2)$, two vectors U and V :

$$G(U, V, A) = (1 + UVA^2) / (1 - U^2)(1 - V^2)(1 - UV) \times (1 - UA^2)(1 - VA^2). \quad (14)$$

(d) $SU(2) \times SU(2)$, a (10) spinor U , a (01) spinor V , a (11) quartet W :

$$G(U, V, W, A, B) = [(1 - WAB)^{-1} + UVW(1 - UVW)^{-1}] \times [(1 - UA)(1 - VB)(1 - W^2)] \times (1 - UWB)(1 - VWA)^{-1}. \quad (15)$$

The indices of the dummies A, B are the $SU(2) \times SU(2)$ representation labels of the tensors.

(e) $SU(3)$, (1, 1) octet U :

$$G(U, A_1, A_2) = (1 + U^2 A_1 A_2 + U^4 A_1^2 A_2^2) \times [(1 - UA_1 A_2)(1 - U^2)(1 - U^3)] \times (1 - U^3 A_1^3)(1 - U^3 A_2^3)^{-1}. \quad (16)$$

This generating function is closely related so that for $SU(3)$ scalars in the enveloping algebra of G_2 .²

We turn to the problem of determining a generating function for multiplets of a subgroup H occurring in IR's of a group G . Start with the character

$\chi_{\mu_1, \dots, \mu_{l_G}}(\eta_1, \dots, \eta_{l_H})$ of the group G . It depends on only l_H variables η because the projection corresponding to the reduction $G \supset H$ has been carried out on the coordinates η in weight space. We may write

$$\chi_{\{\mu\}}(\eta) = \xi_{\{\mu\}}(\eta) / \Delta_G(\eta). \quad (17)$$

The G -representation labels μ_1, \dots, μ_{l_G} in $\xi_{\{\mu\}}$ occur linearly in the exponents of the η 's, with integer coefficients. Now multiply Eq. (17) by $U_1^{\mu_1} U_2^{\mu_2} \cdots U_{l_G}^{\mu_{l_G}}$ and sum over μ_1, \dots, μ_{l_G} ; only geometric series are involved. The result may be written

$$X_{\{U\}}(\eta) = \sum_{\{\mu\}} \left(\prod_i U_i^{\mu_i} \right) \xi_{\{\mu\}}(\eta) / \Delta_G(\eta). \quad (18)$$

It is a generating function for subgroup weights in the IR's of the group G . Now proceed as before. Multiply $X_{\{\mu\}}(\eta)$ by $\Delta_H(\eta)$ [the division of $\sum_{\{\mu\}} (\prod_i U_i^{\mu_i}) \xi_{\{\mu\}}(\eta)$ by $\Delta_G(\eta) / \Delta_H(\eta)$ should be done explicitly, although the details are complicated except in relatively simple cases] and by $\sum_{\{\lambda\}} \Pi_i \eta_i^{M_i - 1} A_i^{\lambda_i}$. Finally add all η -residues inside the unit circles. The result is a generating function $G(U_1, \dots, U_{l_G}, A_1, \dots, A_{l_H})$ for subgroup multiplets ($\lambda_1, \dots, \lambda_{l_H}$) in group IR's (μ_1, \dots, μ_{l_G}). If the generating function can be interpreted in terms of an integrity basis we have a solution of the corresponding internal

labeling problem. A few simple examples follow. They agree with the integrity bases given in Refs. 3 and 6.

(i) $SU(3) \supset O(3)$

$$G = (1 + U_1 U_2 A^2) / (1 - U_1 A^2)(1 - U_1^2)(1 - U_2 A^2)(1 - U_2^2). \quad (19)$$

(ii) $G_2 \supset SU(3)$

$$G = [(1 - U_1)^{-1} + U_2 A_1 A_2 (1 - U_2 A_1 A_2)^{-1}] \times [(1 - U_1 A_1)(1 - U_1 A_2)(1 - U_2 A_1)(1 - U_2 A_2)]^{-1}. \quad (20)$$

(iii) $O(7) \supset G_2$

$$G = [(1 - U_1 U_3 A_2)^{-1} + U_2 A_1 (1 - U_2 A_1)^{-1}] \times [(1 - U_3)(1 - U_3 A_1)(1 - U_1 A_1)(1 - U_2 A_2) \times (1 - U_1 U_2 A_2)]^{-1}. \quad (21)$$

U_1, U_2, U_3 are associated respectively with the 7-, 21-, 8-dimensional fundamental IR's of $O(7)$; A_1, A_2 with the 7-, 14-dimensional fundamental IR's of G_2 . The generating function (21) verifies the integrity basis for $O(7) \supset G_2$ states proposed by Wybourne.⁶

3. ELEMENTARY MULTIPLIETS FOR $O(5) \supset SU(2)$ STATES

Identical particles in the $l=2$ shell may be described in terms of $O(5)$ basis states reduced according to $O(3) \sim SU(2)$.^{7,8} Actually only the nonspinor IR's of $O(5)$ are needed in the shell problem. We give two solutions of the labeling problem in terms of elementary multiplets, the first valid for all IR's of $O(5)$, the second applicable to integer spins only.

Using the technique described in the preceding section we arrive at the following generating function for $SU(2)$ weights contained in IR's of $O(5)$:

$$F(U_1, U_2, \eta) = \frac{(1 + U_2)(1 + U_1^2 U_2) - U_1 U_2 (\eta^3 + \eta + \eta^{-1} + \eta^{-3})}{(1 - U_1 \eta^3)(1 - U_1 \eta)(1 - U_1 \eta^{-1})(1 - U_1 \eta^{-3})(1 - U_2 \eta^4)(1 - U_2 \eta^2)(1 - U_2 \eta^{-2})(1 - U_2 \eta^{-4})}. \quad (22)$$

The coefficient of $U_1^a U_2^b \eta^c$ in F is the multiplicity of the $SU(2)$ weight b in the IR $(\lambda_1 \lambda_2)$ of $O(5)$.

To derive a generating function for $SU(2)$ multiplets in IR's of $O(5)$, one must multiply Eq. (22) by $(\eta^{-1} - \eta) \times (1 - A\eta)^{-1}$ and add the residues of poles with $|\eta| < 1$. Although straightforward in principle, this is a nontrivial task, and is discussed in the Appendix. The result may be written

$$G(U_1, U_2, A) = [(1 - U_2^3)(1 - U_1^4)(1 - U_2 A^4)]^{-1} \{ [1 + U_1 U_2 A + U_1^2 U_2^2 A + U_1 U_2^2 A^3 + (U_1 U_2 A)^3 + U_1^3 U_2^3 + U_2^3 A^6 + (U_1 U_2 A)^2 (U_2^3 A^4) (U_1^4 U_2^2)] [(1 - U_2^2 A^4)(1 - U_1^4 U_2^2)]^{-1} + [U_1^2 A^2 + U_1^3 A^3 + U_1^2 U_2^2 A^4 + (U_1 A^3)(U_1 U_2 A)^2 + (U_1 A^3)(U_1^2 U_2 A^2) + (U_1 A^3)(U_1 U_2 A)(U_1^2 A^2)] [(1 - U_1 A^3)(1 - U_1^2 A^2)]^{-1} + [U_1 A^3 + U_1 U_2 A^5 + (U_1 U_2 A)(U_1 A^3) + (U_1^2 A^2)(U_2^2 A^4) + (U_1 U_2 A)(U_1 U_2^2 A^3) + (U_2^2 A^4)(U_1 U_2 A)^2] [(1 - U_1 A^3)(1 - U_2^2 A^4)]^{-1} + [(U_1^3 U_2 A) + (U_1^3 U_2^2 A) + U_1^4 U_2 A^2 + (U_1^2 A^2)(U_1^4 U_2^2) + U_1^2 U_2 A^2 + (U_1 U_2 A)^2 + (U_1^3 U_2 A)(U_1 U_2 A) + (U_1 U_2 A)(U_1^2 A^2) + (U_1 U_2 A)(U_1^3 U_2^2 A) + (U_1^2 A^2)(U_1^3 U_2 A) + (U_1 U_2 A)^2 (U_1^3 U_2 A) + (U_1 U_2 A)(U_1^2 U_2 A^2)] [(1 - U_1^2 A^2)(1 - U_1^4 U_2^2)]^{-1} \}. \quad (23)$$

The generating function (23) may be interpreted in terms of nineteen elementary multiplets [the notation is $(\lambda_1 \lambda_2 \lambda)$ where $(\lambda_1 \lambda_2)$ are the IR labels for $O(5)$ and λ the $SU(2)$ label]:

$$(014), (024), (030), (036), (103), (111), (115), (123), (202), (212), (224), (303), (311), (321), (400), (412), (420), (521), (630). \quad (24)$$

The form of Eq. (24) indicates that the following products of elementary multiplets should be discarded, in order to avoid redundant states:

- (024) with any of (212), (224), (303), (311), (412), (521), (202)², (111)(202) or (111)(321);
- (420) with any of (103), (115), (224), (303) or (111)(123);
- (103) with any of (036), (123), (311), (321), (412), (521), (111)³ or (111)(212);
- (202) with any of (321), (123), (630), (036), (115) or (111)³; (111)³ with (311);
- (111)² with (123), (212) or (321); (111) with (036), (115), (224), (303), (412), (521) or (630); (111)⁴;
- the product of any two, or the square of any one of (036), (115), (123), (212), (224), (303), (311), (321), (412), (521) or (630).

Stone⁸ has given the branching rules for $O(5) \supset SU(2)$ but has not solved the labeling problem.

The only IR's of $O(5)$ required for spectroscopy are the integer spin IR's (λ_1 even). Retaining the part of G which is even in U_1 yields a generating function for integer spin IR's:

$$G'(U_1, U_2, A) = [(1 - U_2^3)(1 - U_1^4)(1 - U_2 A^4)]^{-1} \{ [1 + U_1^3 U_2^3 + U_2^3 A^6 + (U_1^2 U_2^2 A^2)(U_2^2 A^4)(U_1^4 U_2^2)] [(1 - U_2^2 A^4)(1 - U_1^4 U_2^2)]^{-1} + [U_1^2 A^2 + U_1^4 A^6 + U_1^2 U_2^2 A^4 + (U_1^2 A^6)(U_1^2 U_2^2 A^2) + (U_1^2 A^6)(U_1^2 U_2 A^2) + (U_1^2 A^2)(U_1^2 U_2 A^4)] [(1 - U_1^2 A^6)(1 - U_1^2 A^2)]^{-1} \}$$

$$\begin{aligned}
& + [U_1^2 A^6 + U_1^2 U_2 A^8 + U_1^2 U_2 A^4 + U_1^2 U_2^3 A^4 + (U_1^2 A^2)(U_2^2 A^4) + (U_2^2 A^4)(U_1^2 U_2^2 A^2)] [(1 - U_1^2 A^6)(1 - U_2^2 A^4)]^{-1} \\
& + [U_1^4 U_2 A^2 + U_1^2 U_2 A^2 + U_1^2 U_2^3 A^2 + U_1^4 U_2^2 A^2 + U_1^4 U_2^3 A^2 + (U_1^2 A^2)(U_1^2 A_2^2)] [(1 - U_1^2 A^2)(1 - U_1^2 U_2^2)]^{-1}.
\end{aligned} \tag{25}$$

The interpretation of (25) in terms of an integrity basis is immediate. Again there are nineteen elementary multiplets:

$$\begin{aligned}
& (014), (024), (030), (036), (202), (206), (212), (214), (218), (222), \\
& (224), (234), (400), (406), (412), (420), (422), (432), (630).
\end{aligned} \tag{26}$$

Redundant states are avoided if the following products of elementary multiplets are excluded: (024) with any of (202)², (212), (224), (406), (412), (422), (432), (202)(222) or (202)(420); (420) with any of (206), (214), (218), (224), (234) or (406); (206) with any of (036), (212), (422), (432) or (630); (202) with any of (036), (218), (234) or (630); the product of any two or square of any one of (036), (212), (214), (218), (222), (224), (234), (406), (412), (422), (432) or (630).

4. SUBGROUP SCALARS IN GROUP ENVELOPING ALGEBRA

Often it is useful to know all subgroup scalars, besides the Casimir operators of group and subgroups, which are polynomials in the group generators. They commute with the Casimir operators, and so may serve as missing label operators. The operator properties of the generators may be ignored for the purpose of finding these subgroup scalars. We suppose the terms in the polynomials are symmetrized as to order of the factors—an unsymmetrized term differs from the corresponding symmetrized one by a polynomial of lower degree.

We consider three cases, $G_2 \supset SU(2) \times SU(2)$, $O(5) \supset SU(2)$, and $SU(4) \supset SU(2) \times SU(2)$. In each case there are two missing labels, and hence four functionally independent available missing label operators.⁹ Cases with one missing label have been considered earlier.²

(a) $G_2 \supset SU(2) \times SU(2)$

The group generators decompose into two $SU(2)$ vectors, S and T , the subgroup generators, and a (3, 1) subgroup tensor V with eight components. Apart from the subgroup Casimir operators, subgroup scalars correspond one-to-one to even rank (integer spin) tensors formed from the components of V .

A generating function for $SU(2) \times SU(2)$ tensors in the components of V may be found directly by the methods of this article. However, one can also proceed indirectly. Regard the components of V as bases of the defining IR of $SU(8)$. Then tensors of degree λ in V correspond to $SU(2) \times SU(2)$ multiplets in the IR ($\lambda 000000$) of $SU(8)$. Now $SU(2) \times SU(2)$ is not a maximal subgroup of $SU(8)$ but occurs in the chain $SU(8) \supset O(5) \times SU(2) \supset SU(2) \times SU(2)$; hence the problem may be solved in two steps. The generating function for $O(5) \times SU(2)$ multiplets contained in ($\lambda 000000$) IR's of $SU(8)$ is easily seen to be

$$\begin{aligned}
& [(1 - V^2)(1 - V^2 U_2)(1 - V U_1 B)]^{-1} \\
& = (1 - V^2)^{-1} \sum_{mn} V^{m+2n} U_1^m U_2^n B^m,
\end{aligned} \tag{27}$$

where the factors $U_1^m U_2^n B^m$ correspond to the IR ($mn; m$) of $O(5) \times SU(2)$. Now let

$$G(U_1, U_2, A) = \sum_{mnp} U_1^m U_2^n A^p N_{mnp}, \tag{28}$$

be the generating function for $SU(2)$ IR's contained in

$O(5)$ IR's; G is given explicitly by Eq. (23). We see that to convert (27) to a generating function F for $SU(2) \times SU(2)$ tensors formed from the components of V it is necessary only to replace $U_1^m U_2^n$ by $\sum_p A^p N_{mnp}$. The result is

$$\begin{aligned}
F(V, A, B) & = (1 - V^2)^{-1} \sum_{mnp} V^{m+2n} A^p B^m N_{mnp} \\
& = (1 - V^2)^{-1} G(VB, V^2, A).
\end{aligned} \tag{29}$$

For our purpose, forming subgroup scalars, we want only the part of F which is even in V . That means using G' , Eq. (25) in place of G in Eq. (29). We also replace $A \rightarrow S^{1/2}$, $B \rightarrow T^{1/2}$:

$$F'(V, S, T) = (1 - V^2)^{-1} G'(VT^{1/2}, V^2, S^{1/2}). \tag{30}$$

The exponents of V, S, T in the expansion of F' represent the degrees of the various scalars in the (3, 1) tensor V and in the $SU(2) \times SU(2)$ generators S and T . The exponents of S and T are all integral. There is no need to list the elementary scalars here, since they correspond closely to the elementary multiplets (26). An $O(5) \supset SU(2)$ elementary multiplet (abc) is interpreted as a $G_2 \supset SU(2) \times SU(2)$ scalar ($a + 2b, \frac{1}{2}c, \frac{1}{2}a$). The $SU(2) \times SU(2)$ Casimir operators (0, 2, 0) and (0, 0, 2) and the G_2 Casimir operator (2, 0, 0) must of course be added to the list obtained from (26). The elementary multiplet (030) becomes (600), the sixth degree Casimir operator of G_2 .

Branching rules for $G_2 \supset SU(2) \times SU(2)$ have been given by Stone⁸ and Mandel'tsveig.¹⁰

(b) $O(5) \supset SU(2)$

The group generators decompose into an $SU(2)$ vector L and an $l=3$ tensor U . Since only integer spins are involved, we use conventional l values to label operators; subgroup scalars correspond one-to-one to tensors formed from the components of U . The generating function for the tensors is found by the methods of this article. After some tedious algebra we find the generating function for scalars to be

$$\begin{aligned}
G(U, L) & = [(1 - L^2)(1 - U^2)(1 - U^4)(1 - U^6)(1 - UL^3)(1 - U^2 L^4)]^{-1} \\
& \times \{ [(U^2 L^2)^2 + U^3 L^3 + U^4 L^5 + U^6 L^3 + U^7 L^5 \\
& + (U^2 L^2)(U^3 L^4) + (U^2 L^2)(U^5 L^2) + (U^3 L^4)(U^5 L^2)] \\
& \times (1 - U^2 L^2)^{-1} + [1 + U^2 L^2 + U^3 L + U^3 L^4 + U^3 L^6 + U^4 L^2 \\
& + U^4 L^3 + U^5 L + U^5 L^2 + U^6 L^4 + U^6 L^3 + U^7 L + U^7 L^2]
\end{aligned}$$

$$\begin{aligned}
& + U^8 L + U^3 L^2 + U^{10} L + U^{12} L + U^{15} + (U^{10})(U^3 L^3) \\
& + (U^2 L^2)(U^3 L) + (U^3 L)^2 + (U^3 L)^3 + (U^3 L)^4 + (U^3 L)^5 \\
& + (U^3 L)(U^3 L^3 + U^3 L^4 + U^4 L^2 + U^4 L^3 + U^5 L + U^5 L^2 \\
& + U^5 L^4 + U^6 L^3 + U^7 L + U^7 L^2 + U^8 L + U^9 L^2) \\
& + (U^3 L)^2(U^4 L^2 + U^5 L + U^5 L^2 + U^8 L) \\
& + (U^3 L)^3(U^4 L^2 + U^5 L) + U^5 L(U^3 L^3 + U^4 L^2 + U^5 L^4 \\
& + U^8 L) + (U^3 L)(U^3 L^3)(U^5 L) + (U^{10})(U^3 L^4)(U^5 L^2) \\
& \times (1 - U^{10})^{-1}. \quad (31)
\end{aligned}$$

There are twenty-eight elementary scalars [the notation is (ab) where a and b are the degrees in U and L]:

$$\begin{aligned}
& (02), (13), (20), (22), (24), (31), (33), (34), (36); \\
& (40), (42), (43), (45), (51), (52), (54), (60), (63)_1, (63)_2, \\
& (71), (72), (75), (81), (92), (10, 0), (10, 1), (12, 1), (15, 0).
\end{aligned}$$

The Casimir operators of group and subgroup correspond to (20), (40), (02). There are two missing labels, and hence four functionally independent missing label operators; this is consistent with the fact that, apart from Casimir operators, the denominator of each term of (31) contains four factors.

To avoid redundant scalars the following products of elementary scalars should be avoided:

$$\begin{aligned}
& (22) \text{ with any of } (36), (42), (43), (51), (54), (63)_2, (71), \\
& \quad (72), (81), (92), (10, 1), (12, 1), (15, 0); \\
& (22)^2 \text{ with } (31) \text{ or } (10, 0); (10, 0) \text{ with } (45), (75) \text{ or } (63)_1; \\
& (31) \text{ with } (36), (45), (63)_1, (75), (10, 1), (12, 1) \text{ or } (15, 0); \\
& (31)^2 \text{ with } (22), (33), (34), (43), (54), \\
& \quad (63)_2, (71), (72) \text{ or } (92); \\
& (31)^3 \text{ with } (52) \text{ or } (81); (31)^4 \text{ with } (42) \text{ or } (51); (31)^6; \\
& (51) \text{ with } (34), (36), (43), (45), (52), (63)_1, (63)_2, \\
& \quad (71), (72), (75), (92), (10, 1), (12, 1) \text{ or } (15, 0); (51)^2; \\
& (31)(51) \text{ with } (42), (54) \text{ or } (81);
\end{aligned}$$

the product of any two or square of any one of (33), (34), (36), (42), (43), (45), (52), (54), (63)₁, (63)₂, (71), (72), (75), (81), (92), (10, 1), (12, 1) or (15, 0) with the exception of (34)(52) which is permitted.

(c) $SU(4) \supset SU(2) \times SU(2)$

The generating function for subgroup scalars was derived first by Miller,¹¹ and published with applications to nuclear physics by Quesne.¹² Incidentally, the generating function can be found more simply. The $SU(4)$ generators, decomposed according to $SU(2) \times SU(2)$, consist of a $(1, 1)$ tensor Q and the $SU(2) \times SU(2)$ generators S and T . Regard the nine components of Q as the basis of the defining representation of $SU(9)$. Then the scalars, apart from S^2 and T^2 , correspond to $SU(2) \times SU(2)$ multiplets in IR's $(\lambda 000000)$ of $SU(9)$. Now $SU(2) \times SU(2)$ is not maximal but occurs in the chain $SU(9) \supset SU(3) \times SU(3) \supset SU(2) \times SU(2)$, so the problem can be solved in two steps. The generating function for IR's of

$SU(3) \times SU(3)$ contained in symmetric $SU(9)$ IR's is

$$F(Q, A_1, B_1, A_2, B_2) = [(1 - Q^3)(1 - QA_1A_2)(1 - Q^2B_1B_2)]^{-1}, \quad (32)$$

where the coefficient of $Q^a(A_1A_2)^b(B_1B_2)^c$ is the number of times the IR (ab, ab) occurs in the IR (λ) . Since the branching rules for $SU(3) \supset O(3) \sim SU(2)$ are known [see Eq. (19)], the rest is straightforward.

We give the generating function in a form which has positive terms only in the numerator (as first found by Miller):

$$\begin{aligned}
G(Q, S, T) & = [(1 - S^2)(1 - T^2)(1 - Q^2)(1 - Q^3)(1 - Q^4)(1 - QST)]^{-1} \\
& \times [(1 - Q^2S^2)(1 - Q^2T^2)]^{-1} \{ [1 + Q^2ST + Q^3ST \\
& + Q^5S^2T^2 + Q^3S^2T + Q^4ST^2 + Q^5ST^2 + Q^6T^3] \\
& \times (1 - Q^4T^2)^{-1} + [Q^4S^2(1 + Q^2ST + Q^3ST + Q^5S^2T^2) \\
& + Q^3ST^2 + Q^4S^2T + Q^5S^2T + Q^6S^3](1 - Q^4S^2)^{-1} \}. \quad (33)
\end{aligned}$$

The elementary scalars and their redundant products are obvious. The number of denominator factors in each term is nine, i. e., the number of Casimir operators, five, plus twice the number of missing labels.

5. CONCLUSIONS AND COMMENTS

This paper gives a method for converting a generating function for weights with respect to a compact, semi-simple group into the corresponding generating function for IR's.

One application of the method is to $SU(2)$ bases of $O(5)$ IR's, in terms of elementary multiplets. The stretched products of the elementary multiplets, with certain redundant products discarded, define complete, independent bases for $O(5)$ IR's, and thus solve the state labeling problem. But it should be remarked that they do not constitute explicit expressions for the states; they contain admixtures of states belonging to lower group IR's which must be projected out, a straightforward but tedious task. The generating functions (23), (25), apart from defining states, yield explicit formulas for branching rules, in which only positive terms appear. Stone's branching rule,⁸ obtained by a division process, contains negative as well as positive terms. We hope to find elementary multiplets for other group-subgroup combinations of interest in physics.

We have given integrity bases for missing label operators for $G_2 \supset SU(2) \times SU(2)$ and $O(5) \supset SU(2)$. In each case there are two missing labels and four available independent operators. To define bases, at least one pair of commuting missing label operators must be found. A computer program is being written to find such commuting pairs. In the similar $SU(4) \supset SU(2) \times SU(2)$ case, two pairs of commuting operators are already known.¹³

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APPENDIX

The generating function for $O(5) \supset SU(2)$ elementary

multiplets, discussed in Sec. 3, is given by

$$\sum_{\text{res}} (\eta^{-1} - \eta) F(U_1, U_2, \eta) (1 - A\eta)^{-1}, \quad (\text{A1})$$

where \sum_{res} means sum of residues inside the unit circle and $F(U_1, U_2, \eta)$ is given by Eq. (22). $F(U_1, U_2, \eta)$ has poles inside the unit circle at $\eta = U_1$, $\eta^3 = U_1$, $\eta^2 = U_2$, and $\eta^4 = U_2$.

The residue at $\eta = U_1$ is

$$U_1^6 [(1 - U_1^4)(1 - U_1^2)(1 - U_1^2 U_2) \times (U_2 - U_1^4)(1 - U_1 A)]^{-1}. \quad (\text{A2})$$

The sum of the residues at the three poles for which $\eta^3 = U_1$ is

$$\begin{aligned} & \frac{1}{3} \sum_{m=0}^2 U_1^2 (1 + \omega^m U_1^{4/3} + \omega^{2m} U_1^{8/3}) (\omega^m U_1^{4/3} \\ & + U_2 \omega^{2m} U_1^{2/3} + U_2^2) (\omega^{2m} U_1^{8/3} + U_2 \omega^m U_1^{4/3} + U_2^2) \\ & \times (1 + \omega^m U_1^{1/3} A + \omega^{2m} U_1^{2/3} A^2) \\ & \times [(1 - U_1^4)(1 - U_1^2)(U_1^2 - U_2^3)(U_1^4 - U_2^3)(1 - U_1 A^3)]^{-1}, \quad (\text{A3}) \end{aligned}$$

where $\omega = \exp(2\pi i/3)$.

The sum of the residues of the poles at $\eta = \pm U_2^{1/2}$ is

$$\frac{U_2^4 + U_1^2 U_2^3 + U_1 U_2^3 A + U_1 U_2^3 A^2}{(U_1^2 - U_2^3)(1 - U_2)(1 - U_2^3)(1 - U_1^2 U_2)(1 - U_2 A^2)}. \quad (\text{A4})$$

Finally, the sum of the residues of the poles at $\eta = \pm U_2^{1/4}$, $\pm i U_2^{1/4}$ is

$$\begin{aligned} & \frac{1}{4} \sum_{m=0}^3 U_2 \{ (-i)^m U_2^{3/4} + (-1)^m U_1 U_2^{1/2} + i^m U_1^2 U_2^{1/4} + U_1^3 \} \\ & \times \{ i^m U_2^{3/4} + (-1)^m U_1 U_2^{3/2} + (-i)^m U_1^2 U_2^{3/4} + U_1^3 \} \\ & \times \{ 1 + i^m U_2^{1/4} A + (-1)^m U_2^{1/2} A^2 + (-i)^m U_2^{3/4} A^3 \} \\ & \times \{ 1 + (-1)^m U_2^{3/2} \} \\ & \times [(U_2 - U_1^4)(U_2^3 - U_1^4)(1 - U_2)(1 - U_2^3)(1 - U_2 A^4)]^{-1}. \quad (\text{A5}) \end{aligned}$$

The generating function for $O(5) \supset SU(2)$ multiplets is the sum of (A2), (A3), (A4), and (A5). The sum must now be reduced to a relatively simple form.

Before proceeding with this simplification, we recall that the generating function for $G_2 \supset SU(2) \times SU(2)$ labeling operators is

$$F'(V, S, T) = \frac{1}{2} [F(V, S, T) + F(-V, S, T)], \quad (\text{A6})$$

where

$$\begin{aligned} F(V, S, T) = & [(1 - S^2)(1 - T^2)]^{-1} \sum_{\text{res}} (\eta^{-1} - \eta)(\xi^{-1} - \xi) \\ & \times [(1 - V\eta^3 \xi)(1 - V\eta \xi)(1 - V\eta^{-1} \xi)(1 - V\eta^{-3} \xi) \\ & \times (1 - V\eta^3 \xi^{-1})(1 - V\eta \xi^{-1})(1 - V\eta^{-1} \xi^{-1})(1 - V\eta^{-3} \xi^{-3}) \\ & \times (1 - S^{1/2} \eta)(1 - T^{1/2} \xi)]^{-1}. \quad (\text{A7}) \end{aligned}$$

The summand in (A7) has poles inside the ξ -unit circle at $\xi = V\eta^3$, $V\eta$, $V\eta^{-1}$, and $V\eta^{-3}$. Summing the residues of these poles we find, after some simplification,

$$F'(V, S, T) = (1 - V^2)^{-1} G'(VT^{1/2}, V^2, S^{1/2}), \quad (\text{A8})$$

thus verifying relationship (30) derived in the text.

The first step in the simplification of the sum (A2) + (A3) + (A4) + (A5) is to determine the common denomi-

nator. To do this we set up a computer program to calculate the sum for arbitrary real positive values of U_1 , U_2 , and A . We then search for poles of the form $(1 - U_1^\alpha U_2^\beta A^\gamma)^{-1}$ by giving U_1 , U_2 , and A random values with the constraint

$$U_1^\alpha U_2^\beta A^\gamma = 1 - \epsilon, \quad (\text{A9})$$

where ϵ is small. If the quantity $(1 - U_1^\alpha U_2^\beta A^\gamma)G(U_1, U_2, A)$ remains large in spite of constraint (A9) we conclude that $(1 - U_1^\alpha U_2^\beta A^\gamma)$ is a factor in the common denominator. In this way the denominator factors

$$\begin{aligned} & (1 - U_1), (1 - U_2), (1 - U_1^2 U_2), (1 - U_1 A), \\ & (1 - U_1 A^3), (1 - U_2 A^4), (1 - U_2 A^2) \end{aligned} \quad (\text{A10})$$

are determined. A denominator factor $(1 - Q)$ may correspond to a factor $(1 - Q^n)$ in the final result.

The final expression for $G(U_1, U_2, A)$ is to be a sum of terms, each with a polynomial numerator in U_1, U_2, A with positive coefficients, and a denominator containing factors from the set (A10) in the sense explained above. The maximum number of denominator factors is five [two $O(5)$ labels, one $SU(2)$ label, and two "missing" labels]; that is also evident from the sum (A2) + ... + (A5). We assume each term in the final result contains exactly five denominator factors.

There are seven factors in the set (A10), hence twenty-one possible terms in G . The relation of G to the generating function for $G_2 \supset SU(2) \times SU(2)$ scalars implies that $(1 - U_2^3)^{-1}$ may be assumed to be a common factor; it corresponds to the sixth degree G_2 Casimir operator. This reduces the number of possible terms to fifteen.

A further reduction is obtained by determining which pairs of denominator factors can occur in the same term; this is possible because there are three variables, so two constraints of the form (A9) can be imposed. It turns out that the pairs $(1 - U_2 A^2)(1 - U_1 A)$ and $(1 - U_1^2 U_2)(1 - U_1 A^3)$ cannot occur. Hence $G(U_1, U_2, A)$ has an overall factor $[(1 - U_2^3)(1 - U_1)(1 - U_2 A^4)]^{-1}$ and four possible terms with denominators $(1 - U_2 A^2) \times (1 - U_1^2 U_2)$, $(1 - U_2 A^2)(1 - U_1 A^3)$, $(1 - U_1 A)(1 - U_1^2 U_2)$, and $(1 - U_1 A)(1 - U_1 A^3)$; recall that $(1 - Q)^{-1}$ may appear as $(1 - Q^n)^{-1}$ in the final expression.

Next we consider specific limits of G , for example $U_1 A \rightarrow 1$. Then the term (A2) dominates the sum (A2) + ... + (A5). Since an overall factor $(1 - U_2^3)^{-1}$ is expected we write (A2) as

$$\frac{U_1^3 (1 - U_2^3)}{(1 - U_2^3)(1 - U_1^4)(1 - U_1^2 U_2)(U_2 - U_1^4)(1 - U_1 A)}. \quad (\text{A11})$$

No factor $(U_2 - U_1^4)^{-1}$ can occur in the final result. But in the limit $U_1 A \rightarrow 1$ we have

$$(U_2 - U_1^4) = -U_1^4 (1 - U_2 U_1^{-4}) = -U_1^4 (1 - U_2 A^4), \quad (\text{A12})$$

an acceptable denominator factor. Then, in the limit, (A11) becomes

$$\begin{aligned} & -U_1^2 (1 - U_2^3) [(1 - U_2^3)(1 - U_2 A^4)(1 - U_1 A) \\ & \times (1 - U_1^4)(1 - U_1^2)(1 - U_1^2 U_2)]^{-1} \end{aligned}$$

$$\begin{aligned}
&= -U_1^2(1-U_2^3)(1+U_1^2+U_1^4)(1+U_1^2U_2+U_1^4U_2^2) \\
&\times [(1-U_2^3)(1-U_2A^4)(1-U_1A)(1-U_1^4)(1-U_1^6)(1-U_1^6U_2^3)]^{-1} \\
&= U_1^{-4}(1+U_1^2+U_1^4)(1+U_1^2U_2+U_1^4U_2^2)[(1-U_2^3)(1-U_2A^4) \\
&\quad \times (1-U_1A)(1-U_1^4)]^{-1} \{ (1-U_1^6U_2^3)^{-1} - (1-U_1^6)^{-1} \} \\
&= U_1^{-4}(1+U_1^2+U_1^4)[(1-U_2^3)(1-U_2A^4)(1-U_1^4) \\
&\quad \times (1-U_1A)(1-U_1^2U_2)]^{-1} - U_1^{-4}(1+U_1^2U_2+U_1^4U_2^2) \\
&\quad \times [(1-U_2^3)(1-U_2A^4)(1-U_1^4)(1-U_1A)(1-U_1^2)]^{-1}. \quad (A13)
\end{aligned}$$

The first term has a reasonable denominator and the correct sign. The factor U_1^{-4} can be removed by multiplying by $1=(A_1U_1)^4$. The second term has the wrong sign and a double pole at $U_1=1$. Both problems are cleared up with the substitution

$$(1-U_1^2) - [1-U_1^2(U_1A)^{-3}] = -U_1^{-1}A^{-3}(1-U_1A^3). \quad (A14)$$

Proceeding as above, the following limits of $G(U_1, U_2, A)$ are found. The common denominator factor $D=(1-U_2^3)(1-U_2A^4)(1-U_1^4)$ is removed:

$$\begin{aligned}
\lim_{U_1A^{-1}} DG(U_1, U_2, A) \\
&= U_1^2A^6(1+U_1^2+U_1^4)[(1-U_1A)(1-U_1^2U_2)]^{-1} \\
&\quad + U_1^3A^9(1+U_1^2U_2+U_1^4U_2^2) \\
&\quad \times [(1-U_1A)(1-U_1A^3)]^{-1}, \quad (A15)
\end{aligned}$$

$$\begin{aligned}
\lim_{U_1^2U_2^{-1}} DG(U_1, U_2, A) \\
&= (1+U_1U_2A)[(1-U_1^2U_2)(1-U_2A^2)]^{-1} \\
&\quad + U_1A(1+U_1U_2A+U_2A^2) \\
&\quad \times [(1-U_1^2U_2)(1-U_1A)]^{-1}, \quad (A16)
\end{aligned}$$

$$\begin{aligned}
\lim_{U_1A^3-1} DG(U_1, U_2, A) \\
&= (1+U_1^2A^2+U_1^2U_2^2A^4)[(1-U_1A^3)(1-U_2A^2)]^{-1} \\
&\quad + U_1^2(1+U_2A^2+U_2^2A^4) \\
&\quad \times [(1-U_1A^3)(1-U_1A)]^{-1}, \quad (A17)
\end{aligned}$$

$$\begin{aligned}
\lim_{U_2A^2-1} DG(U_1, U_2, A) \\
&= (1+U_1U_2A+U_1^2U_2)[(1-U_2A^2)(1-U_1A^3)]^{-1} \\
&\quad + U_1^3U_2^2A(1+U_1U_2A)[(1-U_2A^2)(1-U_1^2U_2)]^{-1}. \quad (A18)
\end{aligned}$$

Each pair of terms (A15)–(A18) has the form

$$\frac{N_{ab}}{(1-Q_a)(1-Q_b)} + \frac{N_{ac}}{(1-Q_a)(1-Q_c)}. \quad (A19)$$

There are two ways to manipulate these pairs. Any term in N_{ab} or N_{ac} can be multiplied by Q_a^n . Or N_{ab} and N_{ac} can be altered simultaneously according to

$$N_{ab} \rightarrow N_{ab} + N'(1-Q_b), \quad N_{ac} \rightarrow N_{ac} - N'(1-Q_c). \quad (A20)$$

The goal of these manipulations is to make each pair of terms with a common denominator consistent, i.e., we want to obtain

$$N_{ab} = N_{ba}. \quad (A21)$$

The result thus obtained can differ from $DG(U_1, U_2, A)$ by at most a polynomial in U_1, U_2, A . This polynomial is easily determined by computing the difference between the guessed form of $DG(U_1, U_2, A)$ and the true form for selected values of U_1, U_2, A .

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¹⁴The generating function (31), without the factor $[(1-L^2)(1-U^2)]^{-1}$, may be interpreted also as defining elementary multiplets for $(\lambda 00)$ IR's of $O(7)$, reduced according to $O(3)$. Such states are of interest in connection with nuclear octupole vibrations.

Gel'fand lattice polynomials and irreducible representations of $U(n)$

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A finite difference equation defines the exponential of a square tableau, extension of the usual Gel'fand pattern. These exponentials or " K powers" are homogeneous polynomials useful in the theory of group representations. The theory of these polynomials is developed, and some important addition and multiplication theorems are deduced. The application to the group $U(n)$ gives explicitly the Gel'fand states for $n = 4$, and it is conjectured that the given relation is true in general for any dimension. The matrix elements with respect to this basis are calculated for $n = 3$ and the Clebsch-Gordan decomposition of the n product of $U(2)$ is also given.

1. INTRODUCTION AND NOTATION

The theory of linear representations of the unitary group $U(n)$ is still of constant interest in many physical calculations. The knowledge of the explicit Gel'fand states or the matrix elements of irreducible representations of $U(n)$ is of considerable importance to the atomic, nuclear, or elementary particle physicist. Although a large amount of literature about Gel'fand states exists,¹⁻⁵ explicit expression for these states or for matrix elements of irreducible representations of unitary group are still unknown for arbitrary n .

The first fundamental contribution was given by Gel'fand and Zeitlin⁶ and followed by Gel'fand and Graev.⁶ They gave explicitly the matrix elements of the generators of $U(n)$. Alternative approaches were proposed, later on, by Moshinsky⁷ and by Baird and Biedenharn⁸ using the so-called "boson calculus."

The important contribution of Louck⁹⁻¹¹ must also be mentioned. Louck gives the relationships between the initial Gel'fand, Zeitlin, and Graev approach and the boson calculus approach. Louck and Biedenharn,¹¹ using results on totally tensor operators, gave a procedure in order to obtain recurrently all boson polynomials.

On the other hand, connections between group representations and special functions are well known since the work of Cartan,¹² Vilenkin¹³, Miller,¹⁴ and these two fields are progressing together as it can be nicely seen in the Talman¹⁵ book based on Wigner lectures. The theory of group representations gives new addition theorems on special functions but group theory needs appropriate special functions in order to realize their linear homomorphism.

In the simplest case, appropriate operators acting on the hypergeometric function generate the $SU(3)$ states; but for $SU(4)$, $SU(5)$, or $SL(n+3, \mathbb{C})$ more elaborate functions appear: Appell functions, hypergeometric functions ${}_pF_q$, and Lauricella functions.¹⁶⁻¹⁸

The last important improvement in the theory was

given by Henrich¹⁹ introducing in an elegant formulation the Bargmann-Moshinsky spaces.⁷ These spaces, subspaces of a Fock space over a space of matrices, characterize very nicely any particular representation.

All these approaches suffer from the same difficulty: The functions on which the group element or the operator acts cannot be handled easily because they carry a large number of indices labeling the corresponding representations. It is therefore essential, in order to master the indices, to define very concise notation and to develop in itself the algebra of these symbols.

This self-contained work is an attempt in this direction.^{20,21} Homogeneous polynomials with a large number of variables, called Gel'fand lattice polynomials,²² are associated with a double Gel'fand tableau.

The basic definition, mastering the indices, generalizes in a symmetrized and natural way the definition of the classical exponential x^T , where x is now a set of $\binom{2n}{n}$ initial conditions and T is an n by n Gel'fand lattice.

The algebra of these polynomials are developed in detail and some important addition and multiplication theorems are proved. The lattice structure of the Gel'fand tableau and the decomposition of the Gel'fand lattice in elementary components (binary tableau) play a fundamental role in the results obtained. The theory of group representations is connected with the Gel'fand lattice polynomials by replacing the $\binom{2n}{n}$ variables by the $\binom{2n}{n}$ subdeterminants of a matrix of $GL(n, K)$.

Applications of the multiplication theorems to the group $GL(n, K)$ give explicitly the Gel'fand states for $n = 4$ and it is conjectured that the relation is true in general for any dimension. The matrix elements with respect to this basis are calculated for $n = 3$ and the Clebsch-Gordan decomposition of n products of $U(2)$ is also given.

Notation: The following classical symbols are used in

where the $\binom{2n}{n} - 1$ unknowns $d_{I_i}^{j_i}$ are nonnegative integer solutions of a system of n^2 diophantine linear equations (we eliminate the $T \equiv 0$ lattice), and the summation indices are:

$$\begin{aligned} I_i &= \{i_1 < i_2 < \dots < i_i; 1 \leq i_1 \text{ and } i_i \leq n\}, \\ J_i &= \{j_1 < j_2 < \dots < j_i; 1 \leq j_1 \text{ and } j_i \leq n\}. \end{aligned} \quad (9)$$

The decomposition of any GL in terms of these binary lattices will be called a binary expansion. For $n > 1$ the decomposition is, of course, not unique, but the restrictions on the solutions (nonnegative integers) give for any T a finite number of binary expansions. Let us thus call $S = \{d_{I_i}^{j_i}\}$ the set of all solutions of the binary expansion. m_i^j belongs to each BGL and it is therefore obvious that

$$m_i^j = \sum_{I_i} \sum_{J_i} d_{I_i}^{j_i} \quad \text{for each binary decomposition.} \quad (10)$$

We can therefore conclude that the number of binary expansions of any GL is not larger than the number of partitions of the integer m_i^j .

c. Gel'fand lattice with unique binary expansion (GLUB)

The nonunique binary decomposition is the general rule but in some important cases most of the BGL's cannot appear (from symmetry considerations, for instance) and the decomposition is unique. These GL's are called GLUB's (Gel'fand lattice with unique binary expansion).

Let us give some important GLUB's

1. The so-called maximal GL ($T = \circ [m]_n \circ$)

Their binary expansion is

$$\circ [m]_n \circ = \bigoplus_{I_i} (m_i^j - m_{i+1}^{j+1}) \mathbb{I}_{1, \dots, n-i+1, \dots, n}^{n-i+1, \dots, n} \quad (m_{n+1}^n = 0). \quad (11)$$

2. The so-called left (right) semimaximal GL ($T = \circ [m]_{n-1} [m]_n \circ$ or $T = \circ [m]_n [m]_{n-1} \circ$)

$$\begin{aligned} \circ [m]_{n-1} [m]_n \circ &= \bigoplus_{I_i} (m_i^j - m_{i+1}^{j+1}) \mathbb{I}_{1, n-i+2, \dots, n}^{n-i+1, \dots, n} \\ &\quad \bigoplus_{I_i} (m_{i+1}^j - m_{i+1}^{j+1}) \mathbb{I}_{n-i+1, \dots, n}^{n-i+1, \dots, n} \quad (m_{n+1}^n = 0). \end{aligned} \quad (12)$$

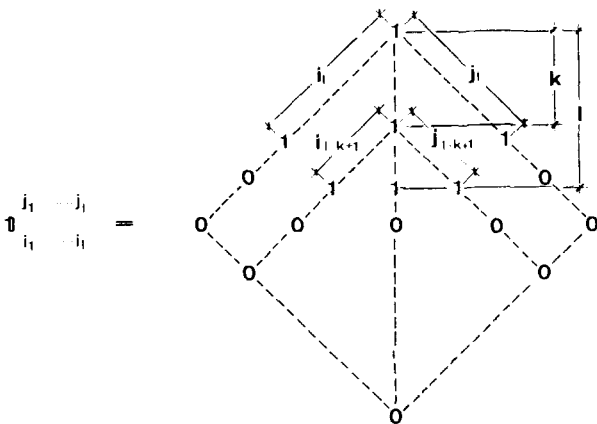


FIG. 2. Binary Gel'fand lattice.

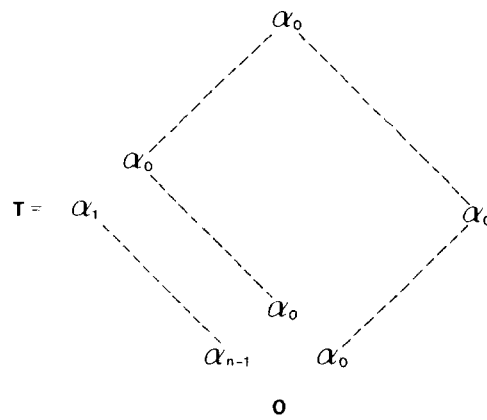


FIG. 3. Peel GLUB.

The binary expansion of the right semimaximal GL is obtained by interchanging the upper and lower indices.

3. The GLUB of Fig. 3, used in the peeling process, has the following decomposition (see C):

$$T = \bigoplus_{i=0}^{n-1} (\alpha_i - \alpha_{i+1}) \mathbb{I}_{1, \dots, (n-i-1), (n-i+1), \dots, n}^{2, 3, \dots, (n-i-1), (n-i+1), \dots, n} \quad (\alpha_n = 0). \quad (13)$$

d. Weights of a GL

To each Gel'fand lattice T corresponds a system of weights $\omega(T)$, defined by the components:

$$\begin{aligned} \omega^j &= s^j - s^{j+1} \quad (\text{right weight}), \\ \omega_i &= s_i - s_{i+1} \quad (\text{left weight}), \end{aligned} \quad (14)$$

where

$$s^j = \sum_{k=1}^{n-j+1} m_k^{j+k-1}, \quad s_i = \sum_{k=1}^{n-i+1} m_{i+k-1}^k, \quad s_{n+1} = s^{n+1} = 0.$$

ω^j (and ω_i) is therefore the difference between the sums of the two adjacent right columns $[m]^{n-j+1}$ and $[m]^{n-j}$ (left columns $[m]_{n-i+1}$ and $[m]_{n-i}$).

In general a given system of weights, with the obvious constraint,

$$\sum_{j=1}^n \omega^j = \sum_{i=1}^n \omega_i \quad (= s^1 = s_1),$$

does not uniquely define a GL.

However, a BGL is uniquely defined by its weights which can take only the value 0 or 1. The building rule for a BGL is the following: $\omega_i = 1$ iff $i \in I_i$ and $\omega^j = 1$ iff $j \in J_i$.

A GLUB is uniquely defined by its weights only if we make precise the "skeleton" components of the GLUB as we can see from the relation

$$\omega(T) = \sum_I d_{I_i}^{j_i} \omega(\mathbb{I}_{I_i}^{j_i}) \quad \text{with } T \text{ a GLUB.} \quad (15)$$

A maximal or semimaximal GL can, for instance, be characterized by their weights.

e. T induction principle

In order to avoid cumbersome notations with multi-indices in each inductive proof, we will always refer

to the following scheme called T inductive reasoning: Let $P(T)$ be a T dependent property, T being a GL. If $P(\underline{0})$ is true and if $P(T')$ true implies $P(T' \oplus \mathbb{1}_{I_l}^{J_l})$ true for all $\binom{2n}{n} - 1$ new GL's, $T' \oplus \mathbb{1}_{I_l}^{J_l}$, then $P(T)$ is true for all T .

B. Exponential of a Gel'fand lattice

a. Finite difference equation

Let K be a zero characteristic commutative field with $\underline{0}$ as null element and $\underline{1}$ as unit element. A 1-1 correspondence can be defined between the set of all BGL's and a subset x of K ,

$$x = \{\underline{1}, x_{I_l}^{J_l} \forall J_l, I_l, 1 \leq l \leq n\},$$

$$\mathbb{1}_{I_l}^{J_l} \rightarrow x_{I_l}^{J_l} \equiv x_{I_l}^{J_l}, \quad 1 \leq l \leq n. \quad (16)$$

Of course, $\underline{1}$ must be associated to the null lattice $\underline{0}$. This application can be extended to the set of all GL,

$$T \rightsquigarrow (T) \in K,$$

via the following finite difference equation

$$(T) = \sum_{\substack{m_l^j \in T \\ (i,j) \neq (1,1)}} (T \ominus T')(T'), \quad (17)$$

and the set x as set of initial conditions. For that reason, the element (T) of K is also noted x^T and is called the " K -power of the set x " or Gel'fand lattice polynomial.

b. Explicit evaluation of x^T

Theorem: For a given set x of initial conditions, the finite difference equation (17) has an unique solution given by

$$x^T = m_1^1! \sum_S \prod_{i=1}^n \prod_{J_l, I_l} \frac{(x_{I_l}^{J_l})^{d_{I_l}^{J_l}}}{d_{I_l}^{J_l}!}, \quad (18)$$

where S is the set of solutions of Eq. (8).

Let us first make some remarks about the solution x^T before proving this theorem.

(i) The following equality is obvious,

$$(x_{I_l}^{J_l})^{d_{I_l}^{J_l}} = x_{I_l}^{J_l} d_{I_l}^{J_l} x_{I_l}^{J_l}. \quad (19)$$

(ii) From the binary expansion of the lattice T , it is clear that

$$m_n^n = d_{12 \dots n}^{12 \dots n}$$

Thus

$$x^T = \binom{m_1^1}{m_n^n} (x_{12 \dots n}^{12 \dots n})^{m_n^n} x^{T \ominus m_n^n \mathbb{1}}. \quad (20)$$

(iii) To each BGL corresponds a monomial of only one variable. To each GLUB corresponds a monomial with r variables if the decomposition of the GLUB in BGL has r terms. To each GL corresponds a homogeneous polynomial of degree m_1^1 with at most $\binom{2n}{n} - 1$ variables and with at most $\binom{2n}{n} - n^2 - 1$ independent summation indices.

It is worthwhile to note that this number is rapidly increasing with n ,

$$\binom{2n}{n} - n^2 - 1 \text{ is } 1, 10, 53 \text{ for } n = 2, 3, 4.$$

(iv) The following relations are obvious [or well known see (f)]:

$$(a) x^{\underline{0}} = \underline{1};$$

$$(b) 0^T = \underline{0}, \text{ where } 0 = \{\underline{1}, x_{I_l}^{J_l} = \underline{0}, \forall J_l, I_l, 1 \leq l \leq n\}, T \neq \underline{0};$$

$$(c) (\lambda x)^T = \lambda^{m_1^1} x^T \quad \lambda \in K;$$

$$(d) x^T x^T = x^T x^T \neq x^{T \oplus T'} \text{ (in general),}$$

$$(x^\nu)^T = \frac{m_1^1!}{(\nu m_1^1)!} \frac{\prod_{i=1}^n \prod_{J_l, I_l} (\nu d_{I_l}^{J_l})!}{\prod_{i=1}^n \prod_{J_l, I_l} (d_{I_l}^{J_l})!} (x)^T,$$

$$\nu \in \mathbf{N}, T \text{ GLUB}, x^\nu = \{\underline{1}, (x_{I_l}^{J_l})^\nu; \forall J_l, I_l, 1 \leq l \leq n\};$$

$$(e) {}^t x^T = x^{tT},$$

where ${}^t T$ is the transposed GL ($m_i^j \in T \iff m_j^i \in {}^t T$) and ${}^t x$ is the set of transposed initial conditions,

$$({}^t x)_{i_1 \dots i_n}^{j_1 \dots j_n} = x_{j_1 \dots j_n}^{i_1 \dots i_n}; \quad (21)$$

(f) The number N of x^T polynomials for a given central column $[m]_n$ is given by the Weyl formula

$$N^{1/2} = d_{[m]_n} = \frac{\prod_{i < j} (m_i^i - m_j^j + j - i)}{\prod_{i=1}^n (n - i)!}. \quad (22)$$

Then the number of BGL $[\binom{2n}{n}]$ can be computed by the Weyl formula. Explicitly,

$$\binom{2n}{n} = \sum_{i=0}^n d_{[1]_i}^2 \text{ with } [1]_i = \left. \begin{matrix} 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{matrix} \right\}^i. \quad (23)$$

Let us now give a detailed constructive proof of the unique Gel'fand lattice polynomial associated with T .

The theorem can be proved via T induction by supposing that (18) is true for all T' with $m_1^1 < m_1^1$. By definition, x^T must in particular verify

$$x^T = \sum_I \sum_{j_1, \dots, j_l} x^{T \ominus \mathbb{1}_{I_1}^{j_1} \dots \mathbb{1}_{I_l}^{j_l}} x_{I_1}^{j_1} \dots x_{I_l}^{j_l} \quad (24)$$

where the summations run over all possible choices of the indices l, i_k, j_k for which $T \ominus \mathbb{1}_{I_1}^{j_1} \dots \mathbb{1}_{I_l}^{j_l}$ is defined. By the induction hypothesis it is clear that

$$x^{T \ominus \mathbb{1}_{I_1}^{j_1} \dots \mathbb{1}_{I_l}^{j_l}} x_{I_1}^{j_1} \dots x_{I_l}^{j_l} = (m_1^1 - 1)! \sum_{S'} \prod_{k=1}^n \left(\prod_{\substack{J_k' \neq J_l \\ I_k' \neq I_l}} \frac{(x_{I_k'}^{J_k'})^{d_{I_k'}^{J_k'}}}{d_{I_k'}^{J_k'}!} \right) \times \frac{(x_{I_1}^{j_1})^{d_{I_1}^{j_1} + 1}}{d_{I_1}^{j_1}!},$$

where S' is the set of all $d_{I_k'}^{J_k'}$ solutions of the binary expansion,

$$T \ominus \mathbb{1}_{I_l}^{j_l} = \bigoplus_{k=1}^n \bigoplus_{\substack{J_k' \neq J_l \\ I_k' \neq I_l}} d_{I_k'}^{J_k'} \mathbb{1}_{I_k'}^{J_k'} \oplus d_{I_l}^{j_l} \mathbb{1}_{I_l}^{j_l}. \quad (26)$$

Let us introduce new summation indices

$$d_{I_k'}^{J_k'} = d_{I_k'}^{J_k'} \text{ if } J_k' \neq J_l \text{ or } I_k' \neq I_l,$$

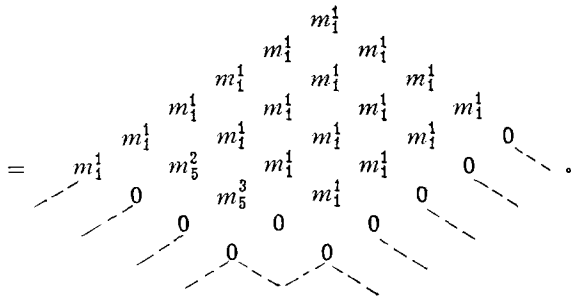
$$d_{I_l}^{j_l} = d_{I_l}^{j_l} + 1 \text{ otherwise.} \quad (27)$$

Thus, with (27), (28) becomes

$$x^T = \sum_{d_{I_k'}^{J_k'}} \prod_{k=1}^n \prod_{J_k'} (x_{I_k'}^{J_k'})^{d_{I_k'}^{J_k'}} \text{ times}$$

and

$$([M_{<2}, m_1^1]_l^3, 3) \begin{matrix} 1, 2, 3, 4 \\ 1, 3, 4, 6 \end{matrix}$$



It is thus obvious that peels are GLUB and that their exponentials are given by

$$([M_{<k}, m_1^1]_l^k)_{I_i}^k = \prod_{s=0}^k \binom{m_1^1}{m_1^1 - s} (x_{I_i}^{J_i(s)})^{m_1^1 + l - s - 1 - m_1^1 - l + s}, \quad (36)$$

$$([M_{<k}, m_1^1]_l^k, j_0)_{I_i}^k = \prod_{s=0}^k \binom{m_1^1}{n_r^{j_0 - s + 1}} (x_{I_i}^{J_i(s)})^{m_1^1 + l - s - m_1^1 - l + s + 1}. \quad (37)$$

D. Particular GL and particular initial conditions

a. Exponential of some particular GL

Let us give explicit solutions of the finite difference equation for some important GL.

1. Maximal GL:

$$x^{* [m]_n} = m_1^1! \prod_{i=1}^n \frac{(x_{n-i+1, n-i+2, \dots, n}^{m_i^1 - m_{i+1}^1})}{(m_i^1 - m_{i+1}^1)!}, \quad (38)$$

where $m_{n+1}^{n+1} = 0$.

2. Semimaximal GL (left or right):

$$x^{* [m]_{n-1} [m]_n} = m_1^1! \prod_{i=1}^n \frac{(x_{n-i+1, n-i+2, \dots, n}^{m_i^1 - m_{i+1}^1})}{(m_i^1 - m_{i+1}^1)!} \frac{(x_{n-i+1, n-i+2, \dots, n}^{m_{i+1}^1 - m_{i+2}^1})}{(m_{i+1}^1 - m_{i+2}^1)!}. \quad (39)$$

where $m_{n+1}^n = m_{n+1}^{n+1} = 0$.

3. l th symmetrical GL:

This GL (see Fig. 4) will be denoted

$$M_{<[m]_n} M_{>} \equiv [M_{<}; m_1^1; M_{>}]_l. \quad (40)$$

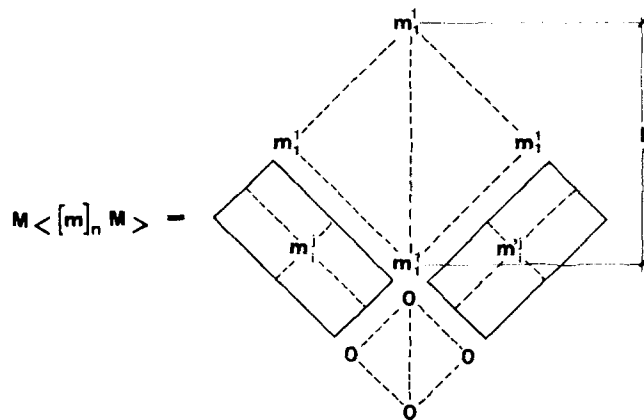


FIG. 4. l th symmetrical Gel'fand lattice.

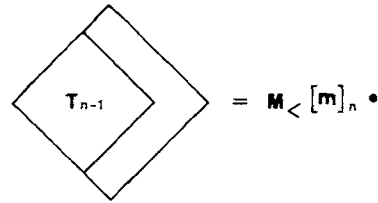


FIG. 5. Partitioned Gel'fand lattice.

It has at most $(2n-l)l$ nonnull elements.

These GL satisfy the following finite difference equations for x^T [notations (T)]:

$$([M_{<}; m_1^1; M_{>}]_l) = \sum_{M_{<}', M_{>}' } ([M_{<} \ominus M_{<}', m_1^1 - m_1^1; M_{>} \ominus M_{>}']_l) \times ([M_{<}', m_1^1; M_{>}']_l). \quad (41)$$

Any GL can be expanded in symmetrical GL, via the peeling procedure in the following way,

$$(T) = \binom{m_1^1}{m_2^1} \circ \circ \binom{m_{n-1}^1}{m_n^1} (T_{[m]_n}), \quad (42)$$

where $(T_{[m]_n})$, the solution of the finite difference equation

$$(T_{[m]_n}) = \sum_{m_i^1 \notin [m]_n} (T_{[m]_n} \ominus T_{[m]_n}')(T_{[m]_n}'), \quad (43)$$

is given by

$$(T_{[m]_n}) = \sum_{\substack{M_{<}^{(i)} \\ M_{>}^{(i)} \\ 2 \leq i \leq n-1}} \prod_{i=1}^n ([M_{<}^{(i)} \ominus M_{<}^{(i+1)}; m_1^1 - m_{i+1}^1; M_{>}^{(i)} \ominus M_{>}^{(i+1)}]_l)$$

with

$$M_{<}^{(1)} = M_{<}, \quad M_{<}^{(n)} = \{m_i^1; m_i^1 = m_n^n\}, \quad (44)$$

$$M_{>}^{(n+1)} = \{m_i^1; m_i^1 = 0\}, \quad m_{n+1}^{n+1} = 0.$$

Indeed, the indices of the central column of $T_{[m]_n}$ now being free indices, can be chosen such that $m_1^1 = m_2^1 = m_2^2$. Because of the betweenness relations, the elements $(m_i^1 - m_{i+1}^1)$ must vanish for $i \geq 3$; the intermediate GL is then first symmetrical. The procedure can be continued with the remaining GL now fixing $m_1^1 = m_2^2 = m_3^3 = m_3^3$; this gives a second symmetrical GL, and so on.

4. Left (right) GL:

These GL's are of the following type:

$$T = M_{<[m]_n} \circ \text{ or } T = \circ [m]_n M_{>}$$

A left GL satisfies the recurrence relation

$$x^{M_{<[m]_n}} = \binom{m_1^1}{m_n^n} \binom{m_1^1 - m_n^n}{m_2^1 - m_n^n} (x_{1, 2, \dots, n}^{1, 2, \dots, n})^n \times (x_1^n)^{m_1^1 - m_2^1} \xi T_{n-1} \ominus m_{n-1}^{n-1}, \quad (45)$$

where T_{n-1} is the GL of dimension $n-1$ obtained from the left GL by elimination of the first right and the last left obliques, as shown in Fig. 5, and ξ is a set of ini-

tial conditions deduced from the set x by the relations

$$\xi_{i_1 \dots i_l}^{j_1 \dots j_l} = \begin{cases} x_{i_1+1}^{j_1} x_{i_2+1}^{j_2} \dots x_{i_l+1}^{j_l} & \text{if } j_1 = 1, \\ x_{i_1+1}^{j_1} x_{i_2+1}^{j_2} \dots x_{i_l+1}^{j_l} & \text{if } j_1 > 1. \end{cases} \quad (46)$$

A similar expression for a right GL is obtained by application of the transposition property.

b. Particular initial conditions

Explicit solutions can also be examined for an arbitrary GL but for particular initial conditions. We consider the following two important cases.

Diagonal initial conditions: Let us call a the set of 2^n nonzero initial conditions obtained in the following way:

$$a = \{ \underline{1}, x_{i_1 \dots i_l}^{j_1 \dots j_l} = \delta_{i_1}^{j_1} \dots \delta_{i_l}^{j_l} a_{i_1 \dots i_l}, 1 \leq l \leq n \} \quad (47)$$

$$a^T = \delta_{M \langle M \rangle} \begin{pmatrix} m_1^1 \\ m_2^1 \end{pmatrix} \dots \begin{pmatrix} m_1^n \\ m_2^n \end{pmatrix} (a_{12 \dots nn})^{m_n^n} \times (a_1)^{m_1^1 - m_2^1} \alpha^{T_{n-1}} \ominus m_n^n \mathbb{1}_{n-1},$$

where

$$\delta_{M \langle M \rangle} = \prod_{1 \leq i < j \leq n} \delta_{m_i^j, m_j^i}$$

T_{n-1} is the truncated GL as before and α is the equivalent of the ξ [Eq. (46)].

Explicitly,

$$\alpha_{i_1 \dots i_l}^{j_1 \dots j_l} = \begin{cases} a_{i_1+1, i_2+1, \dots, i_l+1} & (j_1 = 1, j_2 = n-l+1, \dots, j_l = n-1), \\ a_{i_1+1, \dots, i_l+1} & (j_1 \neq 1, j_1 = n-l). \end{cases} \quad (48)$$

Subdeterminant initial conditions: The set \mathbf{x} of all subdeterminants $x_{i_1 \dots i_l}^{j_1 \dots j_l}$ of a matrix $x = (x_i^j)$ of $M(n, K)$ [in number $\binom{2^n}{n} - 1$] and the element $\underline{1}$ is now chosen as initial conditions.

In this case, some very important properties of the exponentials \mathbf{x}^T must be given.

(i) Let us first consider the canonical injection of $GL(n-1, K)$ in $GL(n, K)$,

$$x_{n-1} = \begin{bmatrix} x_2^2 \dots x_2^n \\ \vdots \\ x_n^2 \dots x_n^n \end{bmatrix} \rightarrow x_n = \begin{bmatrix} \underline{1} & 0 & \dots & 0 \\ 0 & x_2^2 \dots x_2^n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & x_n^2 \dots x_n^n \end{bmatrix} \quad (49)$$

Then

$$\mathbf{x}_{n-1}^{M \langle [m]_{n-1} [m]_{n-1} \rangle} = \delta_{[m]_{n-1} [m]_{n-1}} \begin{pmatrix} m_1^1 \\ m_2^1 \end{pmatrix} \dots \begin{pmatrix} m_1^{n-1} \\ m_2^{n-1} \end{pmatrix} \prod_{i=2}^{n-1} \begin{pmatrix} m_i^{i-1} - m_{i+1}^i \\ m_i^i - m_{i+1}^{i+1} \end{pmatrix} \mathbf{x}_{n-1}^{M \langle [m]_{n-1} \rangle}$$

where

$$\delta_{[m]_{n-1} [m]_{n-1}} = \prod_{i=2}^n \delta_{m_i^{i-1}, m_{i-1}^i} \quad (50)$$

(ii) For any diagonal matrix $a = (a_i^j)$ with $a_i^j = \delta_i^j a_i$, the exponential \mathbf{a}^T is simply given by

$$\mathbf{a}^T = \delta_{M \langle M \rangle} \left[\prod_{i=1}^n \begin{pmatrix} m_i^i \\ m_{i+1}^{i+1} \end{pmatrix} a_i^{\omega_i} \right] \left(\prod_{i < j} \gamma_{ij} \right),$$

where $\omega_i = s_i - s_{i+1}$ are the weight's components of the

left G lattice $M_{\langle [m] \rangle}$.

$$\gamma_{ij} = \begin{pmatrix} m_{i-1}^j - m_i^{j+1} \\ m_i^j - m_{i+1}^{j+1} \end{pmatrix}, \quad m_{n+1}^j = m_n^{j+1} = 0. \quad (51)$$

This is obvious from (47) noticing that here

$$a_{i_1 \dots i_l} = \prod_{k=1}^l a_{i_k}$$

(iii) Finally, the first multiplication theorem can be formulated. For any matrix $x = (x_i^j)$ of $M(n, \mathbb{C})$ and diagonal matrices $a = (\delta_i^j a_i)$ and $a' = (\delta_i^j a_i')$, the following relation is true:

$$(\mathbf{a} \mathbf{x} \mathbf{a}')^T = \left(\prod_{i=1}^n a_i^{\omega_i} \right) \left(\prod_{i=1}^n a_i'^{\omega_i} \right) \mathbf{x}^T, \quad (52)$$

where ω_i and ω_j are the weight's components of T .

E. General properties of x^T

a. Generating function

Let us introduce a set of n^2 elements of K indexed in the following way:

$$\begin{matrix} \lambda_i^1, \mu_i^1, & 1 \leq i, j \leq n, \\ \lambda_i^2, \mu_i^2, & 1 \leq i, j \leq n-1, \\ \dots \dots \dots \\ \lambda_i^k, \mu_i^k, & 1 \leq i, j \leq n-k+1, \\ \dots \dots \dots \\ \lambda_i^n, \mu_i^n, \end{matrix} \quad (53)$$

with the additional constraints $\lambda_i^l = \mu_i^l, 1 \leq l \leq n$.

Then, for a given m_1^1 the following multinomial expansion generates all x^T :

$$\begin{aligned} & \left(\sum_{i=1}^n \sum_{j=1}^{j_i} \lambda_i^j \lambda_{i-1}^j \dots \lambda_{i-1}^j x_{i-1}^{j_i} \mu_i^j \mu_{i-1}^{j-1} \dots \mu_i^{j_i} \right)^{m_1^1} \\ &= \sum_{\substack{(i,j) \neq (1,1) \\ m_i^j}} \left\{ \left(\prod_{l=1}^n \prod_{i=1}^{n-l+1} (\lambda_i^l)^{m_{i+i-1}^l - m_{i+i}^l} \right) \right. \\ & \left. \times x^T \left(\prod_{l=1}^n \prod_{j=1}^{n-l+1} (\mu_i^j)^{m_i^j + j - 1 - m_{i+j}^j} \right) \right\}. \end{aligned} \quad (54)$$

The proof of this formula is inductive on m_1^1 and is immediate by using the finite difference equation.

The following corollary appears obviously by taking all λ_i^j and μ_i^j equal to $\underline{1}$,

$$\left(\sum_{i=1}^n \sum_{j=1}^{j_i} x_{i-1}^{j_i} \right)^{m_1^1} = \sum_{(i,j) \neq (1,1)} x^T. \quad (55)$$

The introduction of the generating function allows us to display some very general properties of x^T .

(i) Let x^T be the K -power of x defined by (54). Then x^T must satisfy the finite difference equation (17) with x as set of initial conditions.

The proof of the converse of theorem (54) is easy by using the fact that $(P)^{m_1^1} = (P)^{m_1^1 - m_{i+1}^i} (P)^{m_{i+1}^i}$.

(ii) The comparison of the two formulas (54) and (55), gives rise to a homogeneity formula.

Let $\Lambda x M$ be the set of initial conditions deduced from

x by the transformations

$$x_{i_1, \dots, i_l}^{j_1, \dots, j_l} \rightarrow \lambda_{i_1}^{j_1} \cdots \lambda_{i_l}^{j_l} x_{i_1, \dots, i_l}^{j_1, \dots, j_l} \mu_{i_1}^{j_1} \cdots \mu_{i_l}^{j_l}. \quad (56)$$

Then

$$(\Delta x M)^T = \left(\prod_{i=1}^n \prod_{j=1}^{n-i+1} (\lambda_{i_1}^{j_1})^{m_{i_1, i-1}^{j_1} - m_{i_1, i}^{j_1}} \right) \times x^T \left(\prod_{i=1}^n \prod_{j=1}^{n-i+1} (\mu_{i_1}^{j_1})^{m_{i_1, i-1}^{j_1} - m_{i_1, i}^{j_1}} \right). \quad (57)$$

(iii) By expanding the first member of (55) in a series with multinomial coefficients, it is clear that for a given m_1^1 the set of x^T forms a partition of the set of the monomials

$$\left(d_{i_1, \dots, i_l}^{j_1, \dots, j_l}, \dots, d_{i_1, \dots, i_l}^{j_1, \dots, j_l} \right) \prod_{i=1}^n \prod_{j=1}^{n-i+1} (x_{i_1}^{j_1})^{d_{i_1}^{j_1}}. \quad (58)$$

All these monomials are linearly independent (for a set x of functionally independent initial conditions). Consequently: For a given m_1^1 and for a set of functionally independent initial conditions, the polynomials x^T are linearly independent on K .

Let us remark that the expansion (55) is a particular case among the various possibilities to summing on a subset of elements of T .

Later, we shall need for example, the following result: Let a be the set of diagonal initial conditions with

$$a_{i_1, \dots, i_l} = \sum_{j_1 < \dots < j_l} \mu_{i_1}^{j_1} \cdots \mu_{i_l}^{j_l} x_{i_1, \dots, i_l}^{j_1, \dots, j_l}.$$

Then

$$a^{M_{\langle [m]_n, t \rangle}} = \sum_{M_{\langle [m]_n, t \rangle}} x^{M_{\langle [m]_n, t \rangle}} \left(\prod_{i=1}^n \prod_{j=1}^{n-i+1} (\mu_{i_1}^{j_1})^{m_{i_1, i-1}^{j_1} - m_{i_1, i}^{j_1}} \right). \quad (59)$$

b. An addition theorem

Let x and y be two sets of initial conditions, and let us define their sum by

$$x + y = \{1, x_{i_1}^{j_1} + y_{i_1}^{j_1}; \forall J_i, I_i, 1 \leq i \leq n\}. \quad (60)$$

Then the following proposition is easily proved by T induction,

$$(x + y)^T = \sum_T \binom{m_1^1}{m_1^1} x^{T \ominus T'} y^{T'}. \quad (61)$$

c. Multiplication theorems

Although multiplications theorems were rigorously established for a wide class of particular cases, no expression is known in the general case. We are only allowed to make the following conjecture:

$$xy^{M_{\langle [m]_n, M \rangle}} = \sum_{\substack{[m']_{n'}^{M'} \\ [m'']_{n''}^{M''}}} x^{M_{\langle [m']_{n'}, M' \rangle}} \frac{1}{\nu(T', T'')} y^{M_{\langle [m'']_{n''}, M'' \rangle}}, \quad (62)$$

where $\nu(T', T'')$ is a constant and where

$$\omega_i' - \omega_i'' = s_i' - s_i'' - (s_i'^{i+1} - s_i''^{i+1}) = 0 \quad 1 \leq i \leq n.$$

But this restriction is not sufficient, as it can be seen in the $n=3$ case. In that case, it is proved (cf. Appendix) that

$$(xy)^{M_{\langle [m]_3, M \rangle}} = \sum_{\substack{[m']_{i'}^{M'} \\ \sigma \tau}} x^{M_{\langle [m']_{i'}, M' \rangle}} \frac{1}{\nu_{[m]_3}(M', \sigma, \tau)} y^{M_{\langle [m']_{i'}, M' \rangle}} \quad (63)$$

where

$$\frac{1}{\nu_{[m]_3}(M', \sigma, \tau)} = \frac{[(m_1^1 - m_2^2)!]^2 (m_1^1 - m_2^2 + 1) (m_1^1 - m_3^3)!}{\binom{m_1^1 - m_2^2}{m_1^1 - m_3^3} \binom{m_2^2 - m_3^3}{m_2^2 - m_3^3}} \times \frac{(-1)^{\sigma+\tau}}{\sigma! \tau!} [(m_1^1 - m_1^1 - \sigma)! (m_2^2 - m_3^3 - \sigma)!] \times (m_1^1 - m_2^2 - \tau)! (m_2^2 - m_3^3 - \tau)! / (m_1^1 - m_3^3 - 2\sigma)! (m_1^1 - m_3^3 - 2\tau)! \times \sum_{\rho} \rho! / [(m_1^1 - m_1^1 - \rho)! (m_2^2 - m_3^3 - \rho)!] \times (m_2^2 - m_3^3 + \rho + 1)! (\rho - \sigma)! (\rho - \tau)! \quad (63)$$

Finally two results for particular cases can be stated for some integers n . The first was obtained before for the exponential of (axa') [Eq. (52)].

The second particular result is true when

$$[m]_n = \{m_1^1, m_2^2 = m_3^3 = \dots = m_n^n\}$$

and it is

$$\binom{m_1^1}{m_n^n} xy^{M_{\langle [m]_n, M \rangle}} = \sum_{[m']_{i'}^{M'}} x^{M_{\langle [m']_{i'}, M' \rangle}} \times \left[\prod_{i=1}^n \binom{m_i^i - m_n^n}{m_i^i - m_n^n} \right]^{-1} y^{M_{\langle [m']_{i'}, M' \rangle}} \quad (64)$$

with

$$m_i^i = m_1^1, \quad m_i^{i+1} = m_n^n$$

3. GROUP REPRESENTATION AND GEL'FAND LATTICE POLYNOMIALS

A. Fock space and Bargmann-Moshinsky representation space

a. Fock space over a space of matrices. Representation space

This section links the Gel'fand lattice polynomials and the representation theory of linear group in a convenient space. These spaces are nicely defined in Henrich and in order to be self consistent we summarize Henrich's essential developments.

Let us consider the vector space $M(n, \mathbb{C})$ with the product

$$(x, y) = \text{Tr}(y^* x). \quad (65)$$

Let γ be the Gaussian measure on $M(n, \mathbb{C})$ defined by

$$d\gamma(x) = C \exp \left[- (x, x) \right] \prod_{i, j=1}^n dR_{ij} x_{ij}^i dI_{ij} x_{ij}^i; \quad x = (x_{ij}^i).$$

Let F_n be the space of analytic functions on $M(n, \mathbb{C})$ such that $\int |f|^2 d\gamma < \infty$. F_n is a Hilbert space, called a Fock space, if we define the following inner product,

$$(f, g) = \int f(x) g^*(x) d\gamma(x). \quad (66)$$

The Fock space is invariant under transformations of the base space which preserve the inner product, e. g., multiplication on the left by a member of $U(n)$. A unitary representation of $U(n)$ L_{ξ} can therefore be defined by the following action,

$$(L_{\xi} f)(x) = f(\xi^* x) \quad (67)$$

with $\xi \in U(n)$.

Bargmann and Moshinsky have indicated a way to

build subrepresentations of L which cover all irreducible representations of $SU(n)$, but the elegant reduction given by Henrich using holomorphic induction is more global:

Let N be the subgroup of $GL(n, \mathbb{C})$ of upper triangular matrices with 1 in the main diagonal,

$$N = \{x \in GL(n, \mathbb{C}), x_i^i = 1, x_i^j = 0, 1 \leq j < i \leq n\}.$$

Let A be the diagonal subgroup of $GL(n, \mathbb{C})$,

$$A = \{a \equiv (a_1 \cdots a_n), a_i \neq 0, 1 \leq i \leq n\}.$$

Definition: $E_{[m]_n}$ is the space of holomorphic functions on $M(n, \mathbb{C})$ which are transformed in the following way under the right action of the group AN of triangular matrices:

$$f(x/a) = \prod_{i=1}^n a_i^{m_i - i + 1} f(x)$$

with

$$l \in N, a \in A, x \in M(n, \mathbb{C}), \quad (68)$$

$$m_i^i \in [m]_n.$$

$B_{[m]_n}$, called the Bargmann–Moshinsky representation space, carries a unitary irreducible representation of $SU(n)$ of dimension $d_{[m]_n}$ given by Weyl's formula [Eq. (22)].

We therefore get a complete list (up to an equivalence) of unitary representations of $SU(n)$ by taking $m_n^n = 0$. Similarly we get a complete list for $U(n)$ by allowing m_n^n to belong now to \mathbb{Z} instead of \mathbb{N} .

b. Reproducing kernel of $B_{[m]_n}$

Defining $K_{[m]_n, y}(x) = K_{[m]_n}(x, y)$ by

$$K_{[m]_n, y} \in B_{[m]_n}, f(y) = (f, K_{[m]_n, y}) \quad \text{if } f \in B_{[m]_n}, \quad (69)$$

we have the following.

Theorem: The reproducing kernel of $B_{[m]_n}$ is

$$K_{[m]_n}(x, y) = k_{[m]_n}(\mathbf{y}^* \mathbf{x})^{\epsilon_{[m]_n}},$$

where $\mathbf{y}^* \mathbf{x}^{\epsilon_{[m]_n}}$ is the maximal G lattice \mathbb{C} power of $\mathbf{y}^* \mathbf{x}$. The explicit value is given by Eq. (38), where

$$k_{[m]_n} = \left[\prod_{i=1}^n \left(\frac{m_i^i}{m_{i+1}^{i+1}} \right) \prod_{i=1}^n (m_i^i + n - i)! \right]^{-1} \times \prod_{1 \leq i < j}^n (m_i^i - m_j^j + j - i). \quad (70)$$

c. Branching operators

The branching operator arises from the embedding of $U(n-1)$ in $U(n)$,

$$\xi_{n-1} = \begin{bmatrix} \xi_1^1 & \cdots & \xi_1^n \\ \xi_2^1 & \cdots & \xi_2^n \\ \vdots & \ddots & \vdots \\ \xi_n^1 & \cdots & \xi_n^n \end{bmatrix} \rightarrow \xi_n = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & \xi_1^1 & \cdots & \xi_1^n \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \xi_n^1 & \cdots & \xi_n^n \end{bmatrix}. \quad (71)$$

If the representation $L^{[m]_n}$ of $U(n)$ is restricted to $U(n-1)$, then according to Weyl's branching law this representation can be decomposed into a direct sum of distinct irreducible representations. Each component is equivalent to $L^{[m]_{n-1}}$ where

$$[m]_{n-1} = \{m_1^1 \leq m_2^2 \leq \cdots \leq m_{i+1}^{i+1} \leq \cdots \leq m_n^{n-1}\},$$

is subject to the ordering relations ("betweenness relations")

$$m_{i+1}^{i+1} \leq m_{i+1}^i \leq m_i^i, \quad 1 \leq i \leq n. \quad (72)$$

This equivalence is realized by a map from $B_{[m]_{n-1}}$ to $B_{[m]_n}$, called a "branching operator" and denoted $R_{[m]_{n-1}}^{[m]_n}$.

$R_{[m]_{n-1}}^{[m]_n}$ intertwines the given representation of $U(n-1)$ on these two spaces,

$$L_{\xi_{n-1}}^{[m]_n} R_{[m]_{n-1}}^{[m]_n} = R_{[m]_{n-1}}^{[m]_n} L_{\xi_n}^{[m]_{n-1}}. \quad (73)$$

$R_{[m]_{n-1}}^{[m]_n}$ is then determined up to a multiplicative constant, because the multiplicities in the branching law are all 0 or 1. We shall choose the constant so that $R_{[m]_{n-1}}^{[m]_n}$ is a partial isometry. The reproducing kernel $R_{[m]_{n-1}}^{[m]_n}(x, y)$ of the branching operator is given by Henrich.¹⁹

Theorem: Let $[m]_n$ and $[m]_{n-1}$ satisfy the betweenness relations. Then there is a branching operator $R_{[m]_{n-1}}^{[m]_n}$ from $B_{[m]_{n-1}}$ to $B_{[m]_n}$, which is an isometry on $B_{[m]_{n-1}}$. The reproducing kernel of $R_{[m]_{n-1}}^{[m]_n}$ is

$$k_{[m]_{n-1}}^{[m]_n}(\mathbf{y}^* \mathbf{x})^{\epsilon_{[m]_{n-1}} [m]_n}. \quad (74)$$

$\epsilon_{[m]_{n-1}} [m]_n$ is the left semimaximal G lattice.

The explicit value is given in Eq. (39) with

$$k_{[m]_{n-1}}^{[m]_n} = \left[\prod_{i=1}^n \left(\frac{m_i^i}{m_{i+1}^{i+1}} \right) \left(\frac{m_{i+1}^{i+1}}{m_{i+1}^i} \right)^{-1} \left[\prod_{i=1}^n (m_{i+1}^{i+1} + n - i + 1)! \right. \right. \\ \times \prod_{i=1}^n (m_i^i + n - i)! \prod_{i < j} (m_{i+1}^{i+1} - m_j^j + j - i - 1)! \\ \left. \left. \times \prod_{i \leq j} (m_i^i - m_{j+1}^j + j - i)! \right]^{-1/2} \right. \\ \times \prod_{i < j} (m_{i+1}^{i+1} - m_{j+1}^j + j - i) \\ \left. \times \prod_{i < j} (m_i^i - m_j^j + j - i)! \prod_{i < j} (m_{i+1}^{i+1} - m_{j+1}^j + j - i)! \right]^{1/2}. \quad (75)$$

d. Gelfand basis vectors

Now, we define an orthonormal basis of each space $B_{[m]_n}$ in the following way: The procedure is inductive on n and assumes that orthonormal bases have been defined for the spaces $B_{[m]_{n-1}}$ such that $R_{[m]_{n-1}}^{[m]_n} \neq 0$. If each basis element is mapped into $B_{[m]_n}$ by the branching operators $R_{[m]_{n-1}}^{[m]_n}$, the resulting vectors form an orthonormal basis of $B_{[m]_n}$. Each basis element is thus of the form:

$$\Gamma = R_{[m]_{n-1}}^{[m]_n} R_{[m]_{n-2}}^{[m]_{n-1}} \cdots R_{[m]_1}^{[m]_2} R_*^{[m]_1}, \quad (76)$$

where $[m]_i$ are chains like in Eq. (4), satisfying the betweenness relations. Here, we could adopt the conventional notation

$$\Gamma \begin{pmatrix} [m]_n \\ \cdots \\ [m]_{n-i}, x \\ \cdots \\ [m]_1 \end{pmatrix}, \quad (77)$$

but for reasons which will appear later, we prefer to

denote the Gel'fand basis element

$$\Gamma(M_{\zeta}[m]_n \cdot, x).$$

A well-known property of the Gel'fand vectors Γ is contained in the following theorem proved in Henrich.¹⁹

Proposition: The Gel'fand vector Γ is an eigenvector of the action of A ; if ω_i is like it is in (14), and $a = (a_1, \dots, a_n)$, then

$$\Gamma(M_{\zeta}[m]_n \cdot, ax) = \prod_{i=1}^n a_i \omega_i \Gamma(M_{\zeta}[m]_n \cdot, x). \quad (78)$$

In connection with Sec. 3 A, we can state the property:

Left G lattice polynomials with central column $[m]_n$ are elements of $B_{[m]_n}$.

We can see that $\mathbf{x}^{M_{\zeta}[m]_n \cdot}$ is a polynomial homogeneous of degree $m_i^1 - m_{i+1}^{i+1}$ in the arguments $x_{i_1 i_2 \dots i_n}^{n-i+1}$. The proof is directly deduced from Proposition (2.2) of Henrich.¹⁹

B. Applications and results

A classical problem of the group's representation theory is to find explicitly an orthogonal basis of the space $B_{[m]_n}$ and then to construct the matrix elements of a linearly irreducible representation of $GL(n, \mathbb{C})$.

The usual method to solving the problem is the "boson calculus" or the technique of the "irreducible tensor operators," but the calculation becomes inextricable for $n \geq 4$. Nevertheless, further results can be obtained owing to the exponential x^T .

a. Basis of $B_{[m]_n}$

Many reasons lead to the following conjecture:

The polynomials $\mathbf{x}^{M_{\zeta}[m]_n \cdot}$ form a basis of $B_{[m]_n \cdot}$ (in general nonorthogonal).

This conjecture is first based on the proven fact that the polynomials $\mathbf{x}^{M_{\zeta}[m]_n \cdot}$ belong to the space $B_{[m]_n}$, and that their number equals the dimension of that space $B_{[m]_n}$. But can it be asserted that all these polynomials are linearly independent? The answer is yes if we can prove the following general result about the linear independence of the \mathbf{x}^T .

Let x be the set of $\binom{\ell^n}{n} - 1$ initial conditions of the finite difference equation (the condition 1 being excluded); let $\mathcal{A}(x)$ be the commutative algebra of polynomials on K with elements of x as variables; let \mathcal{E}_T be the vectorial subspace of $\mathcal{A}(x)$ spanned by the polynomials x^T ; let $\{e_i\}$ be a set of $\binom{\ell^n}{n} - n^2 - 1$ polynomials in the variables x such that $e_i(x) = 0$, those $\binom{\ell^n}{n} - n^2 - 1$ relations being independent; let $\mathcal{J}_{\{e_i\}}$ be the ideal of $\mathcal{A}(x)$ spanned by $\{e_i\}$; then $\mathcal{E}_T \cap \mathcal{J}_{\{e_i\}} = \{0\}$.

This theorem seems to be natural, but we cannot find a rigorous proof.

Nevertheless the above conjecture is true for $n \leq 4$. The basis is in fact orthogonal when n equals 1, 2, or 3 and in the case where $[m]_n = \{m_1^1, m_2^2; m_3^3 = 0; \dots; m_n^n = 0\}$ ($\forall n$), the Gel'fand states are then in Henrich's notations:

(i) $n = 1$:

$$\Gamma(m_1^1; \mathbf{x}) = \frac{1}{(m_1^1!)^{1/2}} \mathbf{x}^{m_1^1}; \quad (79)$$

(ii) $n = 2$:

$$\Gamma(M_{\zeta}[m]_2; \mathbf{x}) = \left[\frac{1}{m_1^1!} \frac{(m_1^1 - m_2^2 + 1)! (m_2^2)! (m_1^1 - m_2^2)! (m_2^2 - m_2^2)!}{(m_1^1 + 1)!} \right]^{1/2} \times \mathbf{x}^{M_{\zeta}[m]_2 \cdot}; \quad (80)$$

(iii) $n = 3$:

$$\Gamma(M_{\zeta}[m]_3; \mathbf{x}) = N \mathbf{x}^{M_{\zeta}[m]_3 \cdot},$$

where

$$N = \frac{1}{m_1^1!} \left[\prod_{i=1}^3 (m_i^i - m_{i+1}^{i+1})! \prod_{i=1}^2 (m_{i+1}^{i+1} - m_{i+2}^{i+2})! \times \prod_{1 \leq i < j \leq 3} (m_i^i - m_j^j + j - i)! \right]^{1/2} \times \left[\frac{(m_2^2 - m_3^3)! (m_3^3 - m_2^2)! (m_2^2 - m_2^2 + 1)}{(m_1^1 + 2)! (m_2^2 + 1)! (m_2^2 - m_3^3 + 1)! (m_1^1 - m_3^3 + 1)!} \right]^{1/2} \quad (81)$$

with $m_3^3 = 0$;

(iv) $[m]_n = \{m_1^1, m_2^2, m_3^3 = 0, \dots, m_n^n = 0\} \quad \forall n$:

$$\Gamma(M_{\zeta}[m]_n; x) = N \mathbf{x}^{M_{\zeta}[m]_n \cdot},$$

where

$$N = \frac{1}{m_1^1!} \left((m_1^1 - m_2^2)! \times \frac{\prod_{j=1}^{n-1} (m_{n-j}^1 - m_{n-j+1}^1)! \prod_{j=0}^{n-2} (m_{n-j}^2 - m_{n-j+1}^2)!}{\prod_{j=1}^{n-1} (m_{n-j}^1 - m_{n-j+2}^2 + 1)!} \right)^{1/2} \times \left[\prod_{j=0}^{n-2} (m_{n-j}^1 - m_{n-j}^2)! \prod_{j=1}^{n-1} (m_{n-j}^1 - m_{n-j+1}^2 + 1) \right]^{1/2} \quad (82)$$

with $m_{n+1}^2 = 0$, and

$$\mathbf{x}^{M_{\zeta}[m]_n \cdot} = m_1^1! \sum_{m_{i_1, i_2}} \prod_{0 \leq i_1 < i_2 \leq n} \frac{(x_{i_1, i_2}^{n-i_1, n})^{d_{i_1, i_2}^{n-1, n}}}{d_{i_1, i_2}^{n-1, n}!}, \quad (83)$$

where

$$x_{0, i_2}^{n-1, n} = x_{i_2}^n,$$

$$d_{i_1, i_2}^{n-1, n} = m_{i_1, i_2} - m_{i_1+1, i_2} - m_{i_1, i_2+1} + m_{i_1+1, i_2+1}.$$

m_{i_1, i_2} are summation indices except for the cases

$$m_{0, i_2} = m_{i_2}^1,$$

$$m_{i_1-1, i_1} = m_{i_1}^2, \quad i_1 > 2,$$

$$m_{i_1, i_1} = m_{i_1, i_1+1},$$

$$m_{i_1, n+1} = 0.$$

(v) If the conjecture is true, this means that there exists a matrix linking this basis to the Gel'fand basis (by the Gram-Schmidt orthogonalization process, for example?). This is true in the $n = 4$ case:

$$\Gamma(M_{\zeta}[m]_3[m]_4; x)$$

$$= N \sum_{\sigma} \frac{(-1)^{\sigma}}{\sigma!} (m_1^1 - m_2^1 + 1)_{\sigma} (m_4^3 - m_4^4 + 1)_{\sigma} \times (m_2^1 - m_4^3 + 2)_{-\sigma} x^{M_{\zeta} \in [m]_3 [m]_4}, \quad (85)$$

where

$$[m]_3' = \{m_2^1 - \sigma, m_3^2, m_4^3 + \sigma\}$$

and the normalization constant is

$$N = \left[\binom{m_1^1}{n_1^1} \prod_{i=1}^3 \binom{m_i^i - m_4^4}{m_{i+1}^i - m_4^4} \binom{m_{i+1}^i - m_4^4}{m_{i+1}^i - m_4^4} \right]^{-1} \left[\nu_{[m]_3} \left(\begin{matrix} m_2^1 \\ m_3^2 \\ m_4^3 \end{matrix}, 0, 0 \right) / \nu_{[m]_3} (M_{\zeta}, 0, 0) A_{[m]_3}^{[m]_4} \right]^{1/2}, \quad (86)$$

where

$$A_{[m]_3}^{[m]_4} = \frac{\prod_{i=1}^4 (m_i^i + 4 - i)! \prod_{i=1}^3 (m_{i+1}^i - m_{i+1}^{i+1})!}{\prod_{1 \leq i < j \leq 4} (m_i^i - m_j^j + j - i)! \prod_{2 \leq i < j \leq 4} (m_i^i - m_j^j - 1 + j - i)!} \times \prod_{2 \leq i < j \leq 4} (m_i^i - 1 - m_j^j + j - i)! \prod_{i=1}^3 (m_i^i - m_{i+1}^i)! \times \prod_{1 \leq i < j \leq 3} (m_i^i - m_{j+1}^j + j - i)!$$

and the $\nu_{[m]_3}(M, \sigma, \tau)$ are defined in (63).

(vi) Finally it can be mentioned that the so-called normalized maximal and semimaximal states are proportional to the maximal and semimaximal GL polynomials. The proportionality constants are:

(α) for the maximal state:

$$\frac{1}{m_1^1!} \prod_{i=1}^n (m_i^i - m_{i+1}^{i+1})! \times \left(\frac{\prod_{j=1}^{n-1} \prod_{k=j+1}^n (m_j^j - m_k^k + k - j)}{\prod_{j=1}^n (m_j^j + n - j)!} \right)^{1/2} (m_{n+1}^{n+1} = 0); \quad (87)$$

(β) for the semimaximal state:

$$\frac{\prod_{i=1}^n (m_i^i - m_{i+1}^{i+1})! \prod_{i=1}^n (m_{i+1}^i - m_{i+1}^{i+1})!}{m_1^1!} \times \left(A_{[m]_{n-1}}^{[m]_n} \right)^{-1/2}, \quad (88)$$

where $m_{n+1}^n = m_{n+1}^{n+1} = 0$;

$$A_{[m]_{n-1}}^{[m]_n} = \frac{\prod_{j=1}^n (m_j^j + n - j)! \prod_{j < k} (m_{j+1}^j - m_k^k + k - j - 1)!}{\prod_{j < k} (m_j^j - m_k^k + k - j)! \prod_{j < k} (m_{j+1}^j - m_{k+1}^k + k - j)!} \times \prod_{j < k} (m_j^j - m_{k+1}^k + k - j)!.$$

b. Matrix elements of the irreducible representations

As a consequence of the above discussion, it can be conjectured that the matrix elements, noted $D_{M_{\zeta} \in [m]_n M}(\mathbf{x})$, of the finite irreducible representation $[m]_n$ of $GL(n, \mathbb{C})$, with respect to the Gel'fand basis, are finite linear combinations of the element \mathbf{x}^T .

This is true in some particular cases. But, before developing those cases, let us remark that if the matrix

\mathbf{x} belongs to $U(n)$, the representation is unitary and irreducible. In that case, the condition $m_n^n \in \mathbb{Z}$ replaces the condition $m_n^n \in \mathbb{N}$, but it is sufficient to extend the definition of the exponential,

$$\mathbf{x}^T = (x_{1,1}^1, x_{1,2}^2, \dots, x_{n,n}^n) \mathbf{x}^{T \ominus (m_n^n \mathbf{1})}. \quad (89)$$

The first obvious particular case is a corollary of the multiplication theorem (64).

(a) The application $GL(n, \mathbb{C}) \rightarrow GL(p, \mathbb{C})$,

$$x \mapsto M_p(x),$$

where $M_p(x)$ is a matrix of order

$$p = \begin{pmatrix} n + m_1^1 - m_n^n - 1 \\ n - 1 \end{pmatrix}$$

whose elements are

$$\left[\prod_{i=1}^n (m_i^i - m_{i+1}^i)! \prod_{j=1}^n (m_i^j - m_{i+1}^{j+1})! \right]^{1/2} \frac{\mathbf{x}^{-1T}}{(m_1^1 - m_n^n)!} \quad (90)$$

with

$$[m]_n = \{m_1^1, m_2^2 = \dots = m_n^n\}$$

is the linear irreducible representation of $GL(n, \mathbb{C})$:

$p \in B_{[m]_n} \rightarrow p' \in B_{[m]_n}$, $p'(y) = p(x^{-1}y)$ with respect to the corresponding Gel'fand basis. Let us note that the exponential \mathbf{x}^T is given in this particular case by

$$(\mathbf{x})^T = \frac{m_1^1!}{(m_n^n)!} (x_{1,1}^1, x_{1,2}^2, \dots, x_{n,n}^n) \sum_{\substack{(m_{(i)}^{(j)}, 1 \leq i, j \leq n)}} \prod_{i,j=1}^n \frac{(x_{ij}^i)^{d_i^j}}{d_i^j!}, \quad (91)$$

where

$$d_i^j = m_{(i)}^{(j)} - m_{(i)}^{(j+1)} - m_{(i+1)}^{(j)} + m_{(i+1)}^{(j+1)},$$

$m_{(i)}^{(j)}$ are summation indices except in the cases

$$m_{(1)}^{(1)} = m_1^1 - m_n^n, \quad m_{(i)}^{(j)} = m_i^j - m_n^n, \quad m_{(i)}^{(n+1)} = m_{(n+1)}^{(j)} = 0.$$

They verify the betweenness relations

$$m_{(i)}^{(j+1)} \leq m_{(i)}^{(j)} \leq m_{(i-1)}^{(j)}. \quad (92)$$

(b) Finally, in the $GL(3, \mathbb{C})$ [resp. $U(3)$] case, the matrix elements of the irreducible representation $[m]_3$ (respectively unitary irreducible representation) are

$$D_{M_{\zeta} \in [m]_3 M}(\mathbf{x}) = \sum_{\sigma} [\nu_{[m]_3}(M_{\zeta}, \sigma, 0)]^{-1/2} \times \mathbf{x}^{*M} \begin{bmatrix} m_1^1 - \sigma \\ m_2^2 \\ m_3^3 + \sigma \end{bmatrix}^M [\nu_{[m]_3}(M, \sigma, 0)]^{-1/2}. \quad (93)$$

c. Product of n representations of $U(2)$

The problem of decomposing the product of n representations of $U(2)$ into a sum of representations of $U(2)$ (Clebsch–Gordan decomposition) was already approached by Henrich.¹⁹ Before we generalize Henrich's work, let us make a short summary of his results.

The Gel'fand basis, in the $n = 2$ case, is formed by the monoms

$$\Gamma(j - m \begin{matrix} 2j \\ 0 \end{matrix}; \mathbf{x}) = \psi_m^j(x_1^2, x_2^2) = [(j - m)! (j + m)!]^{-1/2} (x_1^2)^{j+m} (x_2^2)^{j-m}. \quad (94)$$

The coupling of n angular momenta j_1, \dots, j_n must be described in the space $Q(j_1, \dots, j_n)$, i. e., the space of the polynomials in the $2n$ variables $x_{i_1}^{n-1}, x_{i_2}^n, 1 \leq i_1, i_2 \leq n$, which are homogeneous of degree $2j_i$ in $x_{i_1}^{n-1}, x_{i_2}^n, 1 \leq i \leq n$.

Let $x \in M_n(\mathbb{C})$ be the following matrix:

$$x = \begin{bmatrix} 0 & \cdots & 0 & x_1^{n-1} & x_1^n \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & x_{i_1}^{n-1} & x_{i_1}^n \\ \vdots & & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & x_{n-1}^{n-1} & x_{n-1}^n \end{bmatrix}, \quad (95)$$

$$x_i \equiv (x_{i_1}^{n-1}, x_{i_2}^n).$$

To each matrix $U = (u_i^j)$ of $SU(2)$, there corresponds the matrix of $M_n(\mathbb{C})$

$$U = \begin{bmatrix} 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & 0 \\ 0 & \cdots & 0 & u_1^1 & u_1^2 \\ 0 & \cdots & 0 & u_2^1 & u_2^2 \end{bmatrix}. \quad (96)$$

Then the action of $SU(2)$ on $Q(j_1, \dots, j_n)$, defined by

$$R_U f(x) = f(xU^*), \quad (97)$$

$$U \in SU(2), \quad f \in Q(j_1, \dots, j_n),$$

is the product

$$D^{j_1} \otimes D^{j_2} \otimes \cdots \otimes D^{j_n},$$

where D^{j_i} is the representation of $SU(2)$, with angular momentum j_i .

Then Henrich proves that all the subrepresentations of $D^{j_1} \otimes \cdots \otimes D^{j_n}$, equivalent to D^j can be found by looking for the invariants in $Q(j_1, \dots, j_n, j)$. That is, if $\{f_\sigma\}$ is a complete orthonormal system of invariants in $Q(j_1, \dots, j_n)$, then the generalized Clebsch-Gordan coefficients are given by the following development

$$f(x) = \sum_{m_1, \dots, m_n} \begin{pmatrix} m_1 m_2 \cdots m_n \\ j_1 j_2 \cdots j_n \end{pmatrix} \psi_{m_1}^{j_1}(x) \cdots \psi_{m_n}^{j_n}(x), \quad (98)$$

and the normalized vectors, transforming like $\psi_{m_n}^{j_n}$ are given by

$$\begin{aligned} \tilde{\psi}_{m_n}^{j_n} &= (2j+1)^{1/2} \sum_{m_1, \dots, m_{n-1}} \begin{pmatrix} m_1 m_2 \cdots m_{n-1} j_n \\ j_1 j_2 \cdots j_{n-1} m_n \end{pmatrix} \\ &\times \psi_{m_1}^{j_1}(x_1) \cdots \psi_{m_{n-1}}^{j_{n-1}}(x_{n-1}). \end{aligned} \quad (99)$$

Then Henrich gives the following result: The set of the polynomials

$$f_{M \llbracket m \rrbracket_n} \cdot (x) = N^{1/2} \frac{x^{M \llbracket m \rrbracket_n}}{m_1!}, \quad (100)$$

where \mathbf{x} is the set of subdeterminants of the matrix x given in (95)

$$\begin{aligned} \llbracket m \rrbracket_n &= \{m_1 = m_2^2 = j_1 + j_2 + \cdots + j_n, m_3^3 = \cdots = m_n^n = 0\}, \\ m_1^1 + m_{i+1}^2 &= 2(j_1 + j_{i+1} + \cdots + j_n), \\ m_n^1 &= 2j_n, \end{aligned} \quad (101)$$

$$\begin{aligned} N &= \frac{\prod_{i=1}^{n-1} (m_i^1 - m_{i+1}^2)! \prod_{i=2}^{n-1} (m_i^2 - m_{i+1}^3)! \prod_{i=3}^{n-1} (m_i^3 - m_i^4)!}{\prod_{i=1}^{n-1} (m_i^1 - m_{i+2}^2 + 1)!} \\ &\times \prod_{i=1}^{n-1} (m_i^1 - m_{i+1}^2 + 1), \end{aligned}$$

is a complete orthonormal system of invariants in $Q(j_1, \dots, j_n)$. If $j_1 + \cdots + j_n$ is not an integer, then there are nonnull invariants in $Q(j_1, \dots, j_n)$.

Let us now complete those results using the theory of the exponential x^T . Let us expand the polynomial $x^{M \llbracket m \rrbracket_n}$, already given by (83), in terms of the $\psi_{m_i}(x_i)$ functions. Then we obtain after identification with (98):

$$\begin{aligned} & \left(M \llbracket m \rrbracket_n; \begin{matrix} m_1 & \cdots & m_n \\ j_1 & \cdots & j_n \end{matrix} \right) \\ &= \left[N \prod_{i=1}^n (j_i - m_i)! (j_i + m_i)! \right]^{1/2} \\ &\times \sum_{\substack{\alpha_{i_1 i_2} \\ \beta_{i_1 i_2}}} (-1)^{\sum_{i_1 i_2} \beta_{i_1 i_2}} \left(\prod_{1 < i_1 < i_2 < n} (\alpha_{i_1 i_2} - \beta_{i_1 i_2})! \beta_{i_1 i_2}! \right)^{-1}, \end{aligned} \quad (102)$$

with

$$1 \leq i_1 < i_2 \leq n,$$

$$\alpha_{i_1 i_2} = m_{i_1 i_2} - m_{i_1+1, i_2} - m_{i_1, i_2+1} + m_{i_1+1, i_2+1},$$

$$m_{i_1} = m_i^1, \quad (103)$$

$$m_{i-1, i-1} = m_{i-1, i} = m_i^2, \quad i > 2,$$

$$j_i - m_i = \sum_j \beta_{ij} - \sum_j \beta_{ji} + m_i^1 - m_{i+1}^1.$$

The number of independent summation indices is given by $(n-2)^2$, but it can be reduced to $(n-2)$ by use of the binomial theorem.

Nevertheless, it is useful to introduce the "extra quantum" numbers r_i :

$$m_i^1 = j_i + j_{i+1} + \cdots + j_n + r_i,$$

$$m_i^2 = j_{i-1} + j_i + \cdots + j_n - r_{i-1}, \quad (104)$$

$$r_1 = 0, \quad r_2 = j_1, \quad r_n = j_n.$$

Then they must verify the triangle inequalities

$$|r_i - r_{i+1}| \leq j_i \leq r_i + r_{i+1},$$

and we shall note

$$\left[M \llbracket m \rrbracket_n; \begin{matrix} m_1 \cdots m_n \\ j_1 \cdots j_n \end{matrix} \right] = \left[\begin{matrix} m_1 \cdots m_n \\ j_1 \cdots j_n \\ r_1 \cdots r_n \end{matrix} \right]. \quad (105)$$

Finally, the usual equality

$$\sum_{i=1}^n m_i = 0,$$

must hold.

4. CONCLUSIONS AND EXTENSIONS

The theory developed in this work and the results obtained can be divided in two classes according to their independence or their relations with the theory of linear groups.

I. We have introduced a new type of special function:

The Gel'fand lattice polynomials which are homogeneous polynomials of $\binom{2n}{n}$ variables with positive and integer coefficients. These polynomials are defined in two ways: They are solutions of a "natural" finite difference equation and they can also be obtained from a generating function. The tremendous effort to determine explicitly the Gel'fand lattice polynomials when n is larger than 3 is facilitated by a technique we work out: the peeling process. These polynomials have useful properties as can be seen immediately from the results of Part 2.

It is worth noting that the lattice structure and the binary expansion of a Gel'fand lattice is reminiscent of probability theory. It is not difficult to imagine a process of stochastic nature such that the "hierarchical state" of the system is characterized by a Gel'fand lattice and such that an elementary probability is associated with each binary component. The corresponding Gel'fand lattice polynomial will then give the probability of that state.

II. The connection with group theory, which was the starting point of this work, needs more comments. The Gel'fand lattice polynomial now becomes a very complicated function of all subdeterminants of an arbitrary matrix of $GL(n, \mathbb{C})$. The representation space for $U(n)$ being the Bargmann-Moshinsky space $B_{[m]_n}$, it is natural to write a basis of $B_{[m]_n}$ in terms of Gel'fand lattice polynomials.

We have proved that a *left* Gel'fand lattice polynomial is a basis of $B_{[m]_n}$ for $n \leq 4$ and we conjecture that it is true in general. We also obtained, in a particular case, matrix elements of $GL(n, \mathbb{C})$ in terms of Gel'fand lattice polynomials and it is again conjectured that similar developments exist in general.

A generalization of the multiplication theorem as proven in Appendix B would be the key point to confirm our conjectures. In the case $n=3$ we emphasize the essential role of the generating function (54), of the addition theorem (59), and of the diagonal initial conditions (47).

We also obtained, using the preliminary results of Moshinsky⁷ and Henrich,¹⁹ the explicit Clebsch-Gordan coefficients for the decomposition of the Kronecker product of n representations of $SU(2)$.

Extensions: I. It is tempting, as suggested by Henrich²² to try to extend to other simple Lie algebras the Gel'fand lattice polynomials introduced for A_1 . The answer would probably be given using the weight vectors.²³ The scheme for A_1 is supported by the following reasoning: Let π_1, \dots, π_l be the set of fundamental dominant weights which is a basis of the root system of A_1 . To each element of this set corresponds a fundamental representation of A_1 . Explicitly to π_1 corresponds the identity representation $\{n\}$ of dimension n ($n=l+1$), to π_k corresponds the exterior power $\Lambda^k\{n\}$.

To each of these representations corresponds a weight system labeling biunivocally a basis and consequently a double weight system labeling the related matrix elements. A binary Gel'fand lattice is associated with this set of double weight (except **II**). It is therefore possible to reconstruct the general Gel'fand lattice and also the related polynomials.

II. It would be also interesting, on the basis of the work of Wu,¹⁶ to obtain explicit relations between the Gel'fand lattice polynomials and more standard special functions met in the representation theory of $GL(n, \mathbb{C})$. Lauricella's functions would be a good candidate for this connection.

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APPENDIX A: EXAMPLE OF PEELING ($n=2$)

As indicated in the description of the "peeling procedure" we now illustrate the peeling technique in the $n=2$ case.

Let us write explicitly the fundamental difference equation (17),

$$x^T = \sum_{m_1^1, m_1^2, m_2^1, m_2^2} x^{T \oplus T'} x^{T''}, \quad (A1)$$

where

$$T = m_2^1 \begin{matrix} m_1^1 \\ m_1^2 \\ m_2^2 \end{matrix}, \quad T' = m_1^1 \begin{matrix} m_1^1 \\ m_1^2 \\ m_2^2 \end{matrix},$$

$$T \oplus T' = m_2^1 - m_1^1 \begin{matrix} m_1^1 \\ m_1^2 \\ m_2^2 \end{matrix},$$

with the initial conditions

$$1 = x \begin{matrix} 0 & 0 \\ 0 & 0 \end{matrix}, \quad x_1^1 = x \begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix}, \quad x_2^1 = x \begin{matrix} 1 & 0 \\ 0 & 0 \end{matrix},$$

$$x_1^2 = x \begin{matrix} 0 & 1 \\ 0 & 1 \end{matrix}, \quad x_2^2 = x \begin{matrix} 1 & 1 \\ 0 & 1 \end{matrix}, \quad x_{12}^2 = x \begin{matrix} 1 & 1 \\ 1 & 1 \end{matrix}. \quad (A2)$$

Let us consider the following chain $s = \{m_1^1, m_1^2, m_2^2\}$. The peeling lemma gives

$$x^T = \begin{bmatrix} m_1^1 \\ m_2^1 \end{bmatrix} \begin{bmatrix} m_1^2 \\ m_2^2 \end{bmatrix} x^{T_s}, \quad (A3)$$

with

$$T_s = m_2^1 \begin{matrix} m_1^1 \\ m_1^2 \\ m_2^2 \end{matrix}$$

and x^{T_s} is a solution of the equation

$$x^{T_s} = \sum_{m_1^1, m_1^2, m_2^2} x^{T_s \oplus T_s'} x^{T_s''}, \quad T_s' = m_1^1 \begin{matrix} m_1^1 \\ m_1^2 \\ m_2^2 \end{matrix} \quad (A4)$$

In the first step let us choose the arbitrary integers m_1^1, m_1^2, m_2^2 in the following way

$$m_1^1 = m_1^2 = m_2^2 = m_2^1.$$

By the betweenness relation, the summation indices is

now m_2^2 and the equation becomes

$$x^{T_s} = x^{T_s} \ominus m_2^2 \cdot \mathbf{1} x^{m_2^2 \cdot \mathbf{1}}, \quad (\text{A5})$$

where

$$m_2^2 \cdot \mathbf{1} = m_2^2 \begin{matrix} m_2^2 \\ m_2^2 \end{matrix}$$

The last term of (A5) gives, using relation (19),

$$x^{m_2^2 \cdot \mathbf{1}} = (x_{12}^2)^{m_2^2}. \quad (\text{A6})$$

The first term is the solution of the following equation,

$$x^{T_s} = \sum_{m_1^2} x^{T_s \ominus T_{s'}} x^{T_{s'}}, \quad (\text{A7})$$

where T_s and $T_{s'}$ are now given by

$$T_s = m_2^1 \begin{matrix} m_1^1 \\ 0 \end{matrix} m_1^2, \quad T_{s'} = m_2^1 \begin{matrix} m_1^1 \\ 0 \end{matrix} m_1^2.$$

The choice $m_1^1 = m_2^2 = m_1^2$ generates in (A7) two peels x^{T_i} with the following T_i ($i=1, 2$),

$$T_1 = m_2^1 \begin{matrix} m_1^1 \\ 0 \end{matrix} 0, \quad \text{and} \quad T_2 = m_2^1 \begin{matrix} m_1^1 \\ 0 \end{matrix} m_1^1. \quad (\text{A8})$$

Relations (36) or (37) can now be applied and give

$$x^{T_1} = \begin{pmatrix} m_1^1 \\ m_2^1 \end{pmatrix} (x_1^1)^{m_1^1 - m_2^1} (x_2^1)^{m_2^1}, \quad (\text{A9})$$

$$x^{T_2} = \begin{pmatrix} m_1^1 \\ m_2^1 \end{pmatrix} (x_1^2)^{m_1^1 - m_2^1} (x_2^2)^{m_2^1}. \quad (\text{A10})$$

Collecting (A3), (A6), (A8), (A9), and (A10) we obtain the well known ${}_2F_1$ polynomial occurring in the representation theory of $GL(2, \mathbb{C})$, $SL(2, \mathbb{C})$, $U(2)$, and $SU(2)$ ($m_2^1 \geq m_1^1$),

$$x^T = m_1^1! \frac{(x_{12}^2)^{m_2^2}}{m_2^2!} \sum_{\sigma} \frac{(x_1^1)^{m_1^1 - m_2^1 - m_1^2 + m_2^2 + \sigma}}{(m_1^1 - m_2^1 - m_1^2 + m_2^2 + \sigma)!} \times \frac{(x_2^1)^{m_2^1 - m_2^2 - \sigma}}{(m_2^1 - m_2^2 - \sigma)!} \frac{(x_2^2)^{\sigma}}{\sigma!}, \quad (\text{A11})$$

$$= \begin{pmatrix} m_1^1 \\ m_2^1 \end{pmatrix} \begin{pmatrix} m_2^1 \\ m_1^1 \end{pmatrix} \begin{pmatrix} m_1^2 \\ m_2^2 \end{pmatrix} (x_1^1)^{m_1^1 - m_2^1} (x_2^1)^{m_2^1 - m_2^2} \times (x_2^2)^{m_2^2 - m_1^2} (x_{12}^2)^{m_2^2} {}_2F_1 \left(m_2^1 - m_1^1, m_2^2 - m_1^2; m_2^1 - m_1^1 + 1; \frac{x_2^2 x_1^2}{x_1^2 x_2^2} \right). \quad (\text{A12})$$

(If $m_2^1 \leq m_1^1$, we must exchange the indices 1 and 2.)

This result can of course be easily checked solving in this case the Diophantine equation (8) and using the general result (18).

APPENDIX B: MULTIPLICATION THEOREM ($n=3$)

Before we prove this important multiplication theorem in the $n=3$ case, let us make some general comments.

Let x and y be two elements of $GL(n, K)$ and let $\Delta_{xy} M$ be the set of initial conditions defined in (56) with the n^2 constants

$$\{\lambda_i^l, \mu_i^j; \lambda_i^l = \mu_i^1, 1 \leq l \leq n\}. \quad (\text{B1})$$

The following identity is easily shown

$$P_i \equiv \sum_{I_i, J_i} \lambda_{I_i}^1 \lambda_{I_i-1}^2 \cdots, \quad (\text{B2})$$

$$\lambda_{I_i}^i (xy)_{I_i}^{J_i} \mu_{I_i}^{J_i} \mu_{I_i-1}^{J_i-1} \cdots \mu_{I_i}^{J_i} = \sum_{K_i} X^{K_i} Y_{K_i}, \quad 1 \leq l \leq n,$$

with

$$x^{K_i} = \sum_{I_i} \lambda_{I_i}^1 \lambda_{I_i-1}^2 \cdots \lambda_{I_i}^i x_{I_i}^{K_i}, \quad (\text{B3})$$

$$y_{K_i} = \sum_{J_i} \mu_{J_i}^1 \mu_{J_i-1}^2 \cdots \mu_{J_i}^i y_{K_i}^{J_i}.$$

Now from (54) and (57) we have two different expansions for the generating function (let us choose $m_n^i = 0$ in order to simplify the writing),

$$(P)^{m_1^1} = \left(\sum_{i=1}^n P_i \right)^{m_1^1} = \sum_{T/M_1^1} \left\{ \prod_{l=1}^n \prod_{i=1}^{n-l+1} (\lambda_i^l)^{m_{i+l-1}^i - m_{i+l}^i} (xy)^T \times \left(\prod_{l=1}^n \prod_{j=1}^{n-l+1} (\mu_i^j)^{m_{i+j-1}^i - m_{i+j}^i} \right) \right\} = \sum_{\substack{M_1^1 \\ (i,j) \neq 1}} (\Delta(XY))^{M_1^1} \quad (\text{B4})$$

where $\Delta(XY)$ is the set of initial conditions

$$\Delta(XY) = \{X^{K_i} Y_{K_i}, K_i \in \text{set of multi-indices}, 1 \leq l \leq n\}. \quad (\text{B5})$$

The existence of a multiplication theorem implies that it is possible in general to "separate" the X and Y variables in the expression,

$$\Delta(XY)^{M_1^1} = \begin{pmatrix} m_1^1 \\ m_1^2 \end{pmatrix} (X^1 Y_1)^{m_1^1 - m_1^2} \alpha(XY)^{T_{n-1}}, \quad (\text{B6})$$

with $\alpha(XY)$ defined by (48) and the X^{K_i} and Y_{K_i} are related by the usual subdeterminant relationships.

In the $n=3$ case the "separation" problem is relatively easy to solve. First we have

$$\Delta(XY)^{T_3} = \begin{pmatrix} m_1^1 \\ m_1^2 \end{pmatrix} \begin{pmatrix} m_1^2 \\ m_1^3 \end{pmatrix} (X^1 Y_1)^{m_1^1 - m_1^2} (x_{23}^2 y_{23})^{m_1^3} \alpha(XY)^{T_2}, \quad (\text{B7})$$

with

$$T_3 = m_1^3 \begin{matrix} m_1^1 \\ m_1^2 \\ m_1^3 \end{matrix} m_1^2 \begin{matrix} m_1^1 \\ m_1^2 \end{matrix} m_1^3 \begin{matrix} m_1^1 \\ m_1^2 \end{matrix} 0$$

$$T_2 = m'^2_1 - m'^3_2 \quad m'^2_1 - m'^3_2 \\ 0 \quad m^2_2 - m'^3_2,$$

$$\alpha(XY) = \begin{pmatrix} X^2 Y_2 & X^{12} Y_{12} \\ X^3 Y_3 & X^{13} Y_{13} \end{pmatrix}.$$

Let us now define $\Delta(X) = \{X^{K_i}\}$, $\Delta(Y) = \{Y_{K_i}\}$,

$$\alpha(X) = \begin{pmatrix} X^2 & X^{12} \\ X^3 & X^{13} \end{pmatrix}, \quad \alpha(Y) = \begin{pmatrix} Y_2 & Y_{12} \\ Y_3 & Y_{13} \end{pmatrix}.$$

It can be proved, using orthogonality relations between the Clebsch-Gordan coefficients, that the so-called separation formula is valid,

$$\alpha(XY)^R = \sum_{s_1^1 + s_2^2 = r_1^1} (\det \alpha(X))^{s_2^2} \alpha(X)^s \frac{(s_1^1 - s_2^2 + 1) r_1^1!}{(s_1^1 + 1)! s_2^2!} \\ \times \left[\begin{pmatrix} s_1^1 - s_2^2 & s_1^1 - s_2^2 \\ r_2^2 - s_2^2 & r_1^1 - s_2^2 \end{pmatrix} \right]^{-1} \alpha(Y)^s (\det \alpha(Y))^{s_2^2}, \quad (\text{B8})$$

where

$$R = r_2^2 \quad r_1^1 \quad \text{and} \quad S = r_2^2 - s_2^2 \quad r_1^1 - s_2^2 \\ 0 \quad 0 \quad 0 \quad 0$$

The X^{K_i} (respectively Y_{K_i}) are connected by the usual functional relations between subdeterminants:

$$\det(\alpha(X)) = X^2 X^{13} - X^3 X^{12} = X^1 X^{23} - \lambda_1^1 \lambda_3^1 \lambda_2^2 x_{123}^{123}, \quad (\text{B9})$$

$$\det(\alpha(Y)) = Y_2 Y_{13} - Y_3 Y_{12} = Y_1 Y_{23} - \mu_1^1 \mu_3^1 \mu_2^2 y_{123}^{123},$$

Thus:

$$\Delta(XY)^{T_3} = \begin{pmatrix} m_1^1 \\ m_1'^2 \end{pmatrix} \begin{pmatrix} m_1'^1 \\ m_1'^3 \end{pmatrix} \sum_{\substack{s_1^1 + s_2^2 = m_1'^2 - m_1'^3 \\ \sigma, \tau}} \left[\begin{pmatrix} s_1^1 - s_2^2 \\ m_1'^3 - m_1'^2 - s_2^2 \end{pmatrix} \right]^{-1} \\ \times \left[\begin{pmatrix} s_1^1 - s_2^2 \\ m_1'^2 - m_1'^3 - s_2^2 \end{pmatrix} \right]^{-1} (m_1'^2 - m_1'^3)! (s_1^1 - s_2^2 + 1) s_2^2! \\ \times (s_1^1 + 1)! \left\{ (\lambda_1^1 \lambda_3^1 \lambda_2^2 x_{123}^{123})^\sigma \Delta(X)^{T_3} \frac{(-1)^\sigma}{\sigma! (s_2^2 - \sigma)!} \right. \\ \left. \times \left[\begin{pmatrix} m_1^1 - 2\sigma \\ m_1'^2 - s_2^2 - \sigma \end{pmatrix} \begin{pmatrix} m_1'^2 - s_2^2 - \sigma \\ m_1'^3 + s_2^2 - \sigma \end{pmatrix} \right]^{-1} \right\} \\ \times \{\text{symmetrical expression in } Y; \mu_1^1, \tau\}, \quad (\text{B10})$$

where

$$T'_3 = m'^3_1 - \sigma \quad m'^2_1 - s_2^2 - \sigma \quad m'^2_1 - s_2^2 - \sigma \quad m'^3_1 - \sigma \\ m'^3_2 + s_2^2 - \sigma \quad m'^2_2 - \sigma \quad m'^3_2 + s_2^2 - \sigma \\ 0$$

The expansion of $\Delta(X)^T$ [respectively $\Delta(Y)^T$] in K powers of x (respectively y), using Eq. (59), gives Eq. (63) by identification of the λ_i^j , μ_i^j powers in the two developments of (B4).

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A conformal invariant model of localized spinning test particles

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A purely classical model of massless test particle with spin s is introduced as the dynamical system defined by the ten-dimensional $O(4,2)$ co-adjoint orbit with Casimir numbers $(s^2, 0, 0)$. The Mathisson, Papapetrou *et al.* equations of motion in a gravitational field are recovered, and the particle appears to travel on null geodesics. Several implications are discussed.

I. INTRODUCTION

In the conventional special relativistic treatment of "zero rest mass" spinning test particles,¹⁻³ geometrical conformal invariance appears in a somewhat accidental way⁴ [just as for the unexpected $O(4, 2)$ symmetry of the hydrogen atom problem^{5,6}]. It is well known that such particles dwell on a null hyperplane (existence of a wavefront), whence the related problem of localization. There are severe difficulties when trying a general relativistic approach^{2,7} for the massless particle gains one supplementary degree of freedom (localization by means of gravitational scattering).

The aim of this article is an attempt to reconcile, to some extent, localization and geometrical conformal invariance,^{8,9} by introducing a model where we have insisted on *localization along a curve* of space-time for any test particle (with or without spin) and *conformal invariance*¹⁰ as a guiding principle. The model then appears in an unambiguous way. Whether our model (which has already been investigated, at least from one point of view by Mashhoon¹¹) can account for masslessness of spinning test particles seems to be still under dispute, since no clearcut definition of that concept has been proposed so far.

We review in Sec. II a well-known procedure¹² which yields the Mathisson, Papapetrou *et al.* equations of motion of a test particle with spin in a gravitational field.¹³ In order to get a deterministic set of equations of motion, one must impose supplementary conditions on the skew-symmetric spin tensor $S^{\alpha\beta}$, the linear momentum P^α and perhaps the velocity V^α . Let us recall briefly the different possibilities.

As shown by Dixon,¹⁴ the condition $S^{\alpha\beta}P_\alpha = 0$ seems to be more appropriate than the condition $S^{\alpha\beta}V_\alpha = 0$ in the case of massive particles. A "natural" limiting procedure leads to the following conditions for massless particles, $S^{\alpha\beta}P_\alpha = 0$ and $P_\alpha P^\alpha = 0$.^{7,12,15} These are in fact the basic constraints entering the previously quoted conventional model.

On the other hand, according to our program, once assumed that some localized action functional for a spinning test particle [see (5) below] be conformally

invariant, extra conditions, namely $S^{\alpha\beta}V_\alpha = 0$ and $P_\alpha V^\alpha = 0$, readily follow under the sole requirement that $S^{\alpha\beta}$ be singular. It is then straightforward to derive that the particle travels on null geodesics. We claim that Mashhoon's arguments in favor of the latter supplementary conditions are essentially pervaded by conformal invariance assumptions. It must be emphasized that the $O(4, 2)$ invariance can be ruled out in the flat spacetime case. Section III is thus devoted to the construction of the symplectic structure of the space of motions which is shown—in the free particle case—to be symplectomorphic to a certain 10-dimensional coadjoint orbit of the "conformal group" $O(4, 2)$. This, of course, turns out to be no longer an accidental invariance. We get rid, at the same time, of the instability near the zero curvature of those models introduced by Künzle⁷ and Saturnini.¹⁵

In the last section we show that the fundamental hypotheses of Friedmann's cosmologies need not undergo any modification when spin is admitted for cosmological photons.

II. A MODEL OF MASSLESS SPINNING PARTICLE IN THE GRAVITATIONAL FIELD

For a more detailed account, see Ref. 12. In the case of a continuous distribution of matter, the identity of conservation of the energy momentum tensor¹⁶

$$\hat{\partial}_\alpha T^{\alpha\beta} = 0 \quad (1)$$

is a consequence of the "general covariance" principle which states that the completely continuous functional

$$\mathcal{T}(\delta g) = \frac{1}{2} \int_M T^{\alpha\beta} \delta g_{\alpha\beta} \text{vol} \quad (2)$$

must vanish on those perturbations δg of the gravitational potentials which are Lie derivatives with respect to any differentiable vector field with compact support¹⁷; briefly

$$\mathcal{L}_\xi g = 0 \quad \forall \xi \in \mathcal{X}_0(M). \quad (3)$$

As for localized test particles there exists a standard procedure which brings, using (3), the following action functional^{18,19}:

$$\mathcal{T}(\delta g) = \frac{1}{2} \int_\Lambda (T^{\alpha\beta} \delta g_{\alpha\beta} + T^\gamma{}_\alpha \delta \Gamma^\alpha{}_\beta{}^\gamma) dt \quad (4)$$

into the final form

$$\mathcal{T}(\delta g) = \frac{1}{2} \int_\Lambda (P^\alpha V^\beta \delta g_{\alpha\beta} + S^{\alpha\beta} V^\gamma \hat{\partial}_\alpha \delta g_{\beta\gamma}) dt, \quad (5)$$

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where V is the tangent vector to Λ with respect to t . P and S respectively interpreted as the linear momentum and the skew symmetric spin tensor satisfy, in addition, the following universal equations²⁰ (Mathisson, Papapetrou *et al.* equations of motion):

$$\dot{P} = -\frac{1}{2}R(S) \cdot V, \quad (6)$$

$$\dot{S} = P\bar{V} - V\bar{P}. \quad (7)$$

At this stage one may recall that, in the continuous case (2), the *tracelessness* of the Maxwell-Poynting tensor (for photons) or the Weyl energy momentum tensor (for neutrinos) can be expressed equivalently by the following conformal invariance²¹ of the functional T :

$$T(\lambda g) = 0 \quad \forall \lambda \in C_0(M). \quad (8)$$

It now seems reasonable to maintain Eq. (8) even in the case of concentrated distributions of matter. It is then easy to deduce from (5) and (8) that

$$SV = \mu V \quad (9)$$

and

$$\bar{P}V = \dot{\mu} \quad (10)$$

for some real function μ defined on Λ .

Let us, furthermore, assume that the spin is singular (the condition that the spin should have rank 2 is widely accepted as a central prerequisite), namely

$$\det(S) = 0 \quad (S \neq 0). \quad (11)$$

A quick inspection on the spectrum of S shows that whenever $\text{Tr}(S^2) < 0$ at one point of Λ , one gets in view of (7)²²

$$\mu = 0, \quad (12)$$

$$\text{Tr}(S^2) = : -2s^2 = \text{const}, \quad (13)$$

$$\bar{V}V = 0, \quad (14)$$

$$\dot{V} \text{ parallel to } V. \quad (15)$$

The particle *travels on null geodesics* although its (spacelike!²³) linear momentum and its spin are not parallel transported along Λ [(6), (7)]. The quantities

$$\bar{P}\Theta + \frac{1}{2}\text{Tr}\left(S \cdot \frac{\partial\Theta}{\partial X}\right) = \text{const} \quad (16)$$

are conserved as long as $\Theta \in \mathcal{X}(M)$ satisfies

$$\mathcal{L}_\Theta g = \lambda g \quad [\lambda \in C(M)]. \quad (17)$$

[This can be checked using (9)–(12).]

III. SYMPLECTIC STRUCTURE AND CANONICAL O(4,2) INVARIANCE

Let us start with the observation that the constants of motion (16) associated with any conformal Killing vector field Θ of spacetime provide us with 15 conserved quantities in the flat Minkowski spacetime E . More precisely, the general solution $\Theta \in \mathcal{X}(E)$ of

$$\mathcal{L}_\Theta g = \lambda g, \quad \lambda \in C(E),$$

reads²

$$\Theta = \Lambda \cdot X + \Gamma + A(\bar{X}X) - 2X(\bar{A}X) + \alpha X \quad (X \in E), \quad (18)$$

where $\Lambda \in L(E)$ and $\Lambda + \bar{\Lambda} = 0$ (Lorentz rotation), $\Gamma \in E$

(translation), $A \in E$ (special conformal transformations), $\alpha \in \mathbb{R}$ (dilations). We then define the dual conserved quantities (M, P, K, D) by

$$\bar{P}\Theta + \frac{1}{2}\text{Tr}\left(S \cdot \frac{\partial\Theta}{\partial X}\right) = : \frac{1}{2}\text{Tr}(M\Lambda) + \bar{P}\Gamma + \bar{K}A + D\alpha \quad (19)$$

and thus find

$$M = S + X \cdot \bar{P} - P \cdot \bar{X}, \quad (20)$$

$$K = P(\bar{X}X) - 2X(\bar{P}X) - 2S \cdot X, \quad (21)$$

$$D = \bar{P}X. \quad (22)$$

Set²⁴

$$Z : \begin{bmatrix} \Lambda & -\Gamma\sqrt{2} & A\sqrt{2} \\ -\bar{A}\sqrt{2} & -\alpha & 0 \\ \bar{\Gamma}\sqrt{2} & 0 & \alpha \end{bmatrix}, \quad (23)$$

$$\mu : \begin{bmatrix} M & -K/\sqrt{2} & P/\sqrt{2} \\ -\bar{P}/\sqrt{2} & -D & 0 \\ \bar{K}/\sqrt{2} & 0 & D \end{bmatrix}. \quad (24)$$

It is easy to show that $Z \in \mathcal{G}_{4,2}$ [the Lie algebra of $O(4,2)$] and that $\mu \in \mathcal{G}_{4,2}^*$ since the quantity (19) is equal to

$$\frac{1}{2}\text{Tr}(\mu \cdot Z) = : \mu(Z). \quad (25)$$

Let us then consider *the* 10-dimensional coadjoint orbit of $O(4,2)$ $\Omega_{i_0}^*$ defined by the equation (minimal polynomial)

$$\mu^4 + \mu^2 s^2 = 0 \quad (s \in \mathbb{R}^*), \quad (26)$$

which yields the following compatibility relations

$$\det(S) = 0, \quad (11) \quad (27)$$

$$\text{Tr}(S^2) = -2s^2, \quad (13) \quad (28)$$

$$\bar{P} * (S)^2 P = 0. \quad (25) \quad (29)$$

Note that (28) and (27) are in fact respectively interpreted as the *Casimir* numbers of degree 2 and 4 of this orbit. The last one vanishes as can easily be seen on the characteristic polynomial of μ .

As a final remark, the generic element of $\Omega_{i_0}^*$ is in matrix form

$$\begin{bmatrix} 0 & -\chi s & 0 & 0 & 0 & 0 \\ \chi s & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & \eta \\ 0 & 0 & 1 & -\eta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \quad (30)$$

where $\chi^2 = \eta^2 = +1$. $\Omega_{i_0}^*$ is thus the union of four connected components. χ and η are physically interpreted as the helicity and the sign of the energy as usual for massless particles.

We will, however, confine ourselves to the consideration of the connected component of the identity in

$O(4, 2)$ and put $\chi = \eta = +1$. The co-adjoint infinitesimal action

$$\delta\mu := [Z, \mu], \quad Z \in \mathcal{G}_{4,2}, \quad \mu \in \mathcal{G}_{4,2}^* \quad (31)$$

reads

$$\delta M = [\Lambda, M] + (\Gamma \cdot \bar{P} - P \cdot \bar{\Gamma}) - (K \cdot \bar{A} - A \cdot \bar{K}), \quad (32)$$

$$\delta P = \Lambda \cdot P + 2AD - \alpha P - 2M \cdot A, \quad (33)$$

$$\delta K = \Lambda \cdot K - 2\Gamma D + \alpha K - 2M \cdot \Gamma, \quad (34)$$

$$\delta D = \bar{P}\Gamma - \bar{K}A. \quad (35)$$

Define then according to (27)–(29)

$$V_{11} := \{y = (S, P, X); S \in L(E); S + \bar{S} = 0; \det(S) = 0; \\ \text{Tr}(S^2) = -2s^2; P \in E; \bar{P} * (S)^2 P = 0; X \in E\}, \quad (36)$$

which is called the *evolution space*¹ or the space of initial data since each initial condition y defines a “moment” $\mu \in \mathcal{G}_{4,2}^*$ by the application $y \mapsto \mu$ [(20)–(22)].

The *infinitesimal* action of $O(4, 2)$ on V_{11} can be computed bearing in mind that (18) must hold, and by (32)–(35)

$$\delta S = [\Lambda + 2(A \cdot \bar{X} - X \cdot \bar{A}), S] \quad (37)$$

$$\delta P = [\Lambda + 2(A \cdot \bar{X} - X \cdot \bar{A})]P - (\alpha - 2\bar{A}X)P - 2S \cdot A, \quad (38)$$

$$\delta X = \Theta \quad (18). \quad (39)$$

It is well known that every nontrivial co-adjoint orbit Ω of a Lie group can be endowed with a symplectic structure (Ω, σ) (e. g., Ref. 1). In the case of a semi-simple Lie group

$$\sigma(\delta\mu)(\delta'\mu) = \mu([Z, Z']), \quad \mu \in \Omega \subset \mathcal{G}^*, \\ \delta\mu = [Z, \mu], \quad \delta'\mu = [Z', \mu], \quad Z, Z' \in \mathcal{G}. \quad (40)$$

A tedious calculation shows that in the case of $\Omega_{10}^s \subset \mathcal{G}_{4,2}^*$

$$\sigma(\delta\mu)(\delta'\mu) = -(1/s^2) \text{Tr}(\delta S \cdot S \cdot \delta' S) + \overline{\delta X} \delta' P - \overline{\delta' X} \delta P \quad (41)$$

along with (37)–(39). We can hence define a presymplectic structure on V_{11} which may be still denoted by σ without any ambiguity:

$$\sigma(\delta\mu)(\delta'\mu) = : \sigma(\delta y)(\delta' y). \quad (42)$$

The equations of motion $\delta y \in \ker(\sigma)$ are given by

$$\delta S = P \overline{\delta X} - \delta X \bar{P}, \quad (43)$$

$$\delta P = 0, \quad (44)$$

$$\delta X = \tau * (S)^2 \cdot P \quad (\tau \in \mathbb{R}). \quad (45)$$

Define $U_{10} := V_{11}/\ker(\sigma)$. σ is an integral invariant of the distribution $y \mapsto \ker(\sigma)$ and thus

$$\sigma(\delta y)(\delta' y) = : \sigma(\delta x)(\delta' x), \quad (46)$$

where x denotes the class of y . U_{10} is thus a symplectic manifold, the *space of motions*,¹ which uniquely defines a model of “zero rest mass” spinning particle since it can be easily shown to be symplectomorphic to Ω_{10}^s .²⁶

Let us take into account the gravitational interaction. The simplest way of introducing the minimal gravitational coupling is to replace the derivatives δ in (41) by covariant derivatives $\hat{\delta}$. The requirement that σ be still closed leads in fact to the following expression

$$\sigma(\delta y)(\delta' y) = -(1/s^2) \text{Tr}(\hat{\delta} S \cdot S \cdot \hat{\delta}' S) + \overline{\delta X} \hat{\delta}' P \\ - \overline{\delta' X} \hat{\delta} P + \frac{1}{2} \overline{\delta X} \cdot R(S) \cdot \delta' X. \quad (47)$$

The equations of motion read in this case

$$\hat{\delta} S = P \cdot \overline{\delta X} - \delta X \cdot \bar{P}, \quad (48)$$

$$\hat{\delta} P = -\frac{1}{2} R(S) \cdot \delta X, \quad (49)$$

$$\delta X = \tau * (S)^2 \cdot P \quad (\tau \in \mathbb{R}). \quad (50)$$

in full agreement with the previous [(6), (7), (9), (10), (12), (14), (15)] results as soon as one puts $V := (1/\tau)\delta X$.

IV. CONFORMAL PHOTONS AND THE COSMOLOGICAL HYPOTHESES

In the current formulation of homogeneous cosmology, the compatibility of the 3K microwave background and the model of the universe can be expressed by the existence on spacetime of an infinitesimal conformal generator Θ .^{27,28} It can be shown that the fact that matter flows along the orbits of Θ is a consequence of two basic cosmological hypotheses:

- (i) Light rays are null geodesics;
- (ii) the cosmological radiation is an isotropic black body radiation.

Clearly spin is neglected for photons. If spin is taken into account, (14) and (15) apply just as well. The solution to the second hypothesis challenge can be pictured as follows.

Put

$$\Theta = \beta U, \quad (51)$$

where $\beta = 1/kT$ (k is the Boltzmann constant). U is unit, future pointing and geodesic (matter does not experience any net transfer of energy and momentum from the cosmological radiation). (17) yields that $\text{grad } \beta$ is thus parallel to U , whose curl vanishes.

It is then clear that (16) reduces to

$$\bar{P}\Theta = \text{const} \quad (52)$$

just as if spin were absent.

In other words, if the energy of the photon in the matter frame U is expressed in terms of frequency ν via Planck's law, we still have

$$\nu/T = \text{const}. \quad (53)$$

The spin of the photon does not modify the cosmological interpretation of the redshift, in complete accordance with Wien's law which guarantees that the cosmological radiation remains a black body radiation in spite of the change of temperature.

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²R. Penrose and M. A. H. MacCallum, "Twistor Theory: An Approach to the Quantization of Fields and Space-Time," *Phys. Rep. C* **6**, 242 (1973).
³The phase space (or the space of motions¹) endowed with a six-dimensional symplectic manifold structure can be viewed either as a co-adjoint orbit of the (restricted) Poincaré group with vanishing Casimir numbers ($P_\alpha P^\alpha = W_\alpha W^\alpha = 0$ with $W^\alpha = \chi s P^\alpha$, where s stands for the spin and χ ($\chi^2 = +1$) for the helicity or as the normalized twistor space ($Z^\alpha \bar{Z}_\alpha = 2\chi s$) modulo $U(1)$.²
⁴The $O(4, 2)$ action on the space of motions is not equivariant to the $O(4, 2)$ conformal action on spacetime.
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⁸Since it might appear as a fundamental symmetry of physics rather than an accidental one.⁹
⁹R. Penrose, in *Relativistic Symmetry Groups in Group Theory in Non Linear Problems*, edited by A. O. Barut (Reidel, New York, 1972).
¹⁰In the sense that conformal rescalings $g_{\alpha\beta} \rightarrow \Omega^2 g_{\alpha\beta}$ must be physically insignificant. Conformal invariance is here considered on the same footing as the *general covariance principle* on which our investigations heavily rely.
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¹⁴W. G. Dixon, "Dynamics of Extended Bodies in General Relativity, I," *Proc. Roy. Soc. London A* **314**, 499 (1970).
¹⁵P. Saturnini, "Un modèle de particule à spin de masse nulle dans le champ de gravitation," Thèse de 3ème Cycle (Université de Provence, Marseille, 1976).
¹⁶The hat " $\hat{\cdot}$ " denotes the covariant derivative. Vol is the Riemannian volume element of spacetime (M, g) .
¹⁷Or what amounts to the same thing, that any local smooth change of coordinates must be physically insignificant.
¹⁸Actually a first order distribution with support a one-dimensional curve Λ of M , the world line of the particle. Γ is the Riemannian connection with curvature tensor R . t denotes some parameter of Λ .
¹⁹C. Duval and H. P. Künzle, "Dynamics of Continua and Particles from General Covariance of Newtonian Gravitation theory," Preprint 76/849 CPT/CNRS Marseille (France) (to appear).
²⁰For the sake of simplicity, intrinsic geometrical expressions are extensively used. The bar " $\bar{\cdot}$ " denotes the transposition with respect to $g[\bar{V} := g(V)]$. The skew-symmetric spin tensor is identified with an anti-Hermitian linear operator. $\bar{V}R(S)W := -\text{Tr}(S \cdot R(V, W))$ for any vectors V and W . The dot " \cdot " stands for the covariant derivative with respect to the velocity V .
²¹ $C_0(M)$ denotes the set of all differentiable functions of M with compact support.
²²If $\text{Tr}(S^2) \neq 0$ at one point of Λ , (13), (14), (15) still hold. We discard this unphysical possibility since, in this case, S would have nothing to do with an intrinsic angular momentum.
²³This appears as a venial shortcoming of the theory.¹¹
²⁴With respect to a basis of $E \times \mathbb{R}^2$ whose Gram matrix is given by

$$\begin{bmatrix} \mathbb{1}_E & & \\ & 0 & \mathbb{1} \\ & \mathbb{1} & 0 \end{bmatrix} \cdot$$

²⁵ $*(S)^2 = S^2 - \frac{1}{2} \text{Tr}(S^2) \mathbb{1}_E$ [$*(S)$ denotes the usual adjoint of S]. In fact the only polarization $W := *(M) \cdot P = *(S) \cdot P$ turns out to be null.
²⁶It is sufficient to show that the isotropy subgroup of any particular $\mu \in \Omega_0^2$ is connected [$SO(2) \times \mathbb{R}^4$ in that case] [theorem (11.38) in Ref. 1].
²⁷ Θ is interpreted in the framework of statistical mechanics as the (co-) temperature vectorfield. It is assumed to be time-like and future pointing (the time arrow).²⁸
²⁸J. M. Souriau, "Mécanique statistique, groupes de Lie et Cosmologie in Géométrie symplectique et Physique Mathématique," *Coll. Int. C.N.R.S.* (1974).

The moments of the multiple distribution functions

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The equations of moments equivalent to BBGKY and to the master equations are established with the introduction of an appropriate formalism. We end with the deduction of equations generalizing hydrodynamics. This article is limited to the monoparticle populations.

I. INTRODUCTION

Classical statistical mechanics reposes on Liouville's equation,¹ whence the BBGKY² system is deduced by regression and on a hypothesis of irreversibility introduced in the latter. The most famous hypothesis is that of molecular chaos which leads to Boltzmann's equation^{1,3} and with which Chapman,⁴ Enskog,⁵ Burnett^{6,7} and Grad^{7,8} have determined the expressions for the transport coefficients of dilute gases. We owe to Grad^{7,8} a famous method obtained on developing the single distribution function in Hermite tensorial polynomials of the components of the relative velocity vector. The development coefficients are combinations of the distribution function so that, on substituting the approximation of the latter into the integral term of Boltzmann's equation and on making suitable integrations, one obtains the set of equations of fluid mechanics. One then deduces their viscosity and thermal conductivity terms. Like Boltzmann's equation, the main kinetic equations are deduced from BY1 (with possible "manipulations" of BY2 to obtain approximations of the integral term). One may ask if this description suffices for all fluids. Bogoliubov^{7,9} has replied positively to this question for dilute gases but one may doubt that this would obtain for dense gases, plasmas, or liquids. Sandri,^{10,11} on introducing the "master equation" idea, is entirely of this opinion. However, it must be recognized that such a step, above all, runs into difficulties because of the complicated formalism. In particular, Grad's method (mentioned above) is difficult to transpose to higher orders.

On returning to the BBGKY system, we will, in this article, introduce the relative moments of the distribution functions of arbitrary order and, by integration, obtain the general systems of the equations of single (order one) and multiple moments.

II. SPECIAL NOTATION

To arrive at the equations of simple form, it is necessary to introduce a particular notation and convention¹²:

(1) If necessary, we will use the same symbols for the signs and physical quantities as confusion is impossible. Thus n may be used indifferently for a particle density or the sign of the number of a particle.

(2) The signs may be placed below, above, on the right, or on the left. The numbers of the concerned particles are shown above; those on the left characterize a direct relation with the particles; those on the right,

an indirect one. The Cartesian components are shown by signs placed below and on the right. For the applications, it is not necessary to distinguish the variance as the space is properly Euclidean. Thus, ${}^a\mathbf{x}$ and ${}^a\mathbf{w}$ are the position and velocity vectors of the particle of number a which we subsequently call particle a . The components are of the following type: 1x_1 for the first Cartesian component of the position vector of the particle 1; 2w_j for the j th Cartesian component of the velocity vector of the particle 2, These conventions extend to the tensor components. ${}^{11}T_{ij}$ is relative to the particle 1, ${}^{123}T_{ij}$ to the particles 1, 2, and 3,

(3) This notation is accurate but heavy. Now, the BBGKY system of equations is a system of scalar equations obtained on summing over the components of the vectors attached to a whole series of particles. Thus it is interesting to attempt to lighten the notation. To achieve this, we have to use two sets \mathbb{N}^n and \mathbb{I}^n . N is the number of the particles of the population concerned, \mathbb{N}^n is the set of N natural first integers,

$$\mathbb{N}^n = \{1, 2, 3, \dots, r, \dots, N-2, N-1, N\}.$$

\mathbb{I}^n will be the set of the small greek letters completed by N elements: $\mathbb{I}^n = \{\alpha, \beta, \gamma, \dots, \rho, \dots, \xi, \psi, \zeta\}$; the presence of non-fully-written elements is without incidence since the generality of the various reasoning only gives rise to $\alpha, \beta, \gamma, \rho, \xi, \psi, \zeta$.

Let us introduce the bijection h between the two sets, $\mathbb{N}^n \xrightarrow{h} \mathbb{I}^n$, such that

$$h(1) = \alpha, h(2) = \beta, h(3) = \gamma, \dots, h(r) = \rho, \dots, h(N-2) = \xi, h(N-1) = \psi, h(N) = \zeta.$$

The element α is a variable sign which can take each of the Cartesian positions of the particle 1. When it is repeated, we apply Einstein's convention and sum up,

$$A_\alpha B_\alpha = {}^1A_1^1B_1 + {}^1A_2^1B_2 + {}^1A_3^1B_3 = {}^1A \cdot {}^1B.$$

The element β is a variable sign which can take each of the Cartesian positions of both particle 1 and 2. When it is repeated, we sum up to obtain

$$A_\beta B_\beta = {}^1A_1^1B_1 + {}^1A_2^1B_2 + {}^1A_3^1B_3 + {}^1A_1^2B_1 + {}^2A_2^2B_2 + {}^2A_3^2B_3,$$

$$A_\beta B_\beta = {}^1A \cdot {}^1B + {}^2A \cdot {}^2B,$$

and so on for $\gamma, \dots, \rho, \dots, \xi, \psi, \zeta$. Such quantities are come across in classical statistical mechanics. In a general manner, the sign ρ is associated with the r first particles and its repetition implies the summation

over all the components of the r particles,

$$A_\rho B_\rho = {}^1A \cdot {}^1B + {}^2A \cdot {}^2B + \dots + {}^rA \cdot {}^rB,$$

$$T_{\rho\alpha} A_\rho = {}^{11}T_{1\alpha} {}^1A_1 + {}^{11}T_{2\alpha} {}^1A_2 + {}^{11}T_{3\alpha} {}^1A_3 \\ + {}^{21}T_{1\alpha} {}^2A_1 + {}^{21}T_{2\alpha} {}^2A_2 + {}^{21}T_{3\alpha} {}^2A_3 \\ + \dots + {}^{r1}T_{1\alpha} {}^rA_1 + {}^{r1}T_{2\alpha} {}^rA_2 + {}^{r1}T_{3\alpha} {}^rA_3.$$

Lastly, we define the elements of the set $\overline{\Pi}^N$,

where

$$\overline{\Pi}^N = \{\overline{\alpha}, \overline{\beta}, \overline{\gamma}, \dots, \overline{\rho}, \dots, \overline{\xi}, \overline{\psi}\}$$

comprises only $N - 1$ elements of which each is a variable sign taking the three Cartesian values of the particles that are not concerned by their homolog of $\overline{\Pi}^N$, for example, $\overline{\rho}$ concerns and describes the components of the particles $r+1, r+2, \dots, N$; since ρ is relative to the particles $1, 2, \dots, r$. This allows us to write $\forall \rho \in \overline{\Pi}^N \Rightarrow \overline{\rho} \in \overline{\Pi}^N$,

$$A_\zeta B_\zeta = A_\rho B_\rho + A_{\overline{\rho}} B_{\overline{\rho}}.$$

(4) The notation relative to the acceleration vectors, to which the particles are submitted, must be especially adapted if one wishes to arrive at condensed formulas. The interaction force sustained by the i particle under the effect of the particle j is ${}^iX^j$ and the force of external origin is iX . One will note that the signs on the left are relative to the particles sustaining the forces and that the sign on the right are relative to the particles inducing these interactions. For the corresponding acceleration vectors, we suggest the following notations,

$${}^i a^j = \frac{{}^i X^j}{m}, \quad {}^i a^i = \frac{{}^i X}{m}.$$

Thus the acceleration sustained by the number i particle, through the external and interaction forces with the first n particles, is written ${}^i a^{1\dots n} = \sum_{j=1}^{j=n} {}^i a^j$; the symbol $a_p^{1\dots n}$ then represents one of the three components of the acceleration sustained by any one of the first r particles under the effect of the external forces (if number $\in [n, \dots, u]$, and the interaction forces, with the set of particles whose number belongs to $[n, \dots, u]$. Thus, for example,

$$a_p^{n_1 \dots n_u} b_p = \sum_{q=1}^{q=3} \sum_{j=n}^{j=u} \sum_{i=1}^{i=r} {}^i a_q^j b_q.$$

(5) We will end with the signs on showing the sum of the components of a tensor of arbitrary order, obtained by circular permutations of the signs, in the following form,

$$T_{\langle i_1 i_2 \dots i_{q-1} i_q \rangle} = T_{i_1 i_2 \dots i_{q-1} i_q} \\ + T_{i_2 \dots i_{q-1} i_q i_1} + \dots + T_{i_q i_1 i_2 \dots i_{q-1}},$$

for example, we will write:

$$T_{\langle \rho_1 \rho_2 A \rho_3 \rangle} = T_{\rho_1 \rho_2 A \rho_3} + T_{\rho_2 \rho_3 A \rho_1} + T_{\rho_3 \rho_1 A \rho_2}, \\ T_{\rho_1 \langle \rho_2 A \rho_3 \rangle} = T_{\rho_1 \rho_2 A \rho_3} + T_{\rho_1 \rho_3 A \rho_2}, \\ \frac{\partial}{\partial \lambda} (V_{i_1} V_{i_2} \dots V_{i_q}) = V_{\langle i_1 V_{i_2} \dots V_{i_{q-1}} \frac{\partial}{\partial \lambda} V_{i_q} \rangle}$$

(6) Lastly, the phase-space volume of the r particles will be

$$\underline{d^{1\dots r} x} \underline{d^{1\dots r} w} = \underline{d^1 x} \underline{d^2 x} \dots \underline{d^r x} \underline{d^1 w} \underline{d^2 w} \dots \underline{d^r w},$$

with classically $\underline{d^i x} = d^i x_1 d^i x_2 d^i x_3$,

likewise $\underline{d^i w} = d^i w_1 d^i w_2 d^i w_3$.

The principal conventions being established, we can begin the calculations on a population of N particles.

III. THE BBGKY EQUATIONS AND THE MASTER EQUATIONS

On calling $D = D(x_\zeta, w_\zeta, t)$, the phase-space density for a population composed of N identical particles, we define the generic distribution function of rank N such that

$${}^{1\dots N} F = N! D.$$

On multiplying Liouville's equation by $N!$, we establish the N th BBGKY equation,

$$\left(\frac{\partial}{\partial t} + w_\zeta \frac{\partial}{\partial x_\zeta} + a_\zeta^{1\dots N} \frac{\partial}{\partial w_\zeta} \right) {}^{1\dots N} F = 0. \quad (1)$$

The other generic distribution functions ${}^{1\dots r} F$ of rank r (lower than N) are obtained from ${}^{1\dots N} F$,

$${}^{1\dots r} F = \frac{1}{(N-r)!} \int \underline{d^{r+1} x} \underline{d^{r+1} w} \dots \underline{d^N x} \underline{d^N w} {}^{1\dots N} F. \quad (2)$$

To achieve this, it is practical to introduce the operator \hat{r} to write (2),

$${}^{1\dots r} F = \hat{r} {}^{1\dots N} F, \quad \text{with}$$

$$\hat{r} = \frac{1}{(N-r)!} \int \underline{d^{r+1} x} \underline{d^{r+1} w} \dots \underline{d^N x} \underline{d^N w}. \quad (3)$$

One will note that \hat{r} commutes with the operators

$$\frac{\partial}{\partial t}, w_\rho \frac{\partial}{\partial x_\rho}, a_\rho^{1\dots r} \frac{\partial}{\partial w_\rho} \quad [\text{with } \rho = h(r)].$$

To obtain the r th BBGKY equation, let us apply the operator \hat{r} on Eq. (1),

$$\left(\frac{\partial}{\partial t} + w_\rho \frac{\partial}{\partial x_\rho} + a_\rho^{1\dots r} \frac{\partial}{\partial w_\rho} \right) \hat{r} {}^{1\dots N} F \\ + \hat{r} \left(w_{\overline{\rho}} \frac{\partial}{\partial x_{\overline{\rho}}} + a_{\overline{\rho}}^{1\dots N} \frac{\partial}{\partial w_{\overline{\rho}}} \right) {}^{1\dots N} F \\ + \hat{r} a_{\overline{\rho}}^{r+1\dots N} \frac{\partial}{\partial w_{\overline{\rho}}} {}^{1\dots N} F = 0. \quad (4)$$

In Eq. (4), the term

$$\hat{r} \left(w_{\overline{\rho}} \frac{\partial}{\partial x_{\overline{\rho}}} + a_{\overline{\rho}}^{1\dots N} \frac{\partial}{\partial w_{\overline{\rho}}} \right) {}^{1\dots N} F$$

is zero; indeed, since ${}^{1\dots N} F \rightarrow 0$ when the vectors \mathbf{x} or \mathbf{w} tend to their limit values. On the other hand, as the particles are indiscernible, one may write

$$r a_{\overline{\rho}}^{r+1\dots N} \frac{\partial}{\partial w_{\overline{\rho}}} {}^{1\dots N} F = (N-r) \hat{r} a_{\overline{\rho}}^{r+1} \frac{\partial}{\partial w_{\overline{\rho}}} {}^{1\dots N} F$$

or again

$$\int \underline{d^{r+1} x} \underline{d^{r+1} w} (r+1) \hat{\S} a_{\overline{\rho}}^{r+1} \frac{\partial}{\partial w_{\overline{\rho}}} {}^{1\dots N} F$$

according to the recurrence relation drawn from (3), linking \hat{r} to $(r+1)\hat{\S}$,

$$\hat{r} = \frac{1}{(N-r)} \int \underline{d^{r+1} x} \underline{d^{r+1} w} (r+1) \hat{\S}.$$

As $(r+1)\$ and $a_p^{r+1}(\partial/\partial w_p)$ commute, on taking account of (2), we write Eq. (4) as follows:$

$$\left(\frac{\partial}{\partial t} + w_p \frac{\partial}{\partial x_p} + a_p^{1 \dots r} \frac{\partial}{\partial w_p}\right) 1 \dots r F + \int \underline{d^{r+1}x} \underline{d^{r+1}w} a_p^{r+1} \frac{\partial}{\partial w_p} r \dots r+1 F = 0. \quad (5)$$

This equation is BY r —a BBGKY equation of rank r . The BBGKY equations of rank greater than or equal to r constitute a closed system of equations coupled two by two. The determination of $1 \dots r F$ is followed successively by that of $1 \dots r-1 F$, then $1 \dots r-2 F$, ..., then $1 \dots r+1 F$. It should be noted that this manner of calculating $1 \dots r F$ is not unique and that Eq. (1) and the definition (2) of $1 \dots r F$ also suffices. However, Eq. (5) has another interest, generally speaking, the description of a "gas" may be sufficiently minute with $1 \dots r F$, therefore it is desirable to know the equation having the solution $1 \dots r F$; such a specific equation of the "gas" will be worked out by the physicist from BY r with the adapted hypotheses and approximations.

The equation, having the solution $1 \dots r F$, is called the master equation of rank r , ME r in short,

$$\left(\frac{\partial}{\partial t} + w_p \frac{\partial}{\partial x_p} + a_p^{1 \dots r} \frac{\partial}{\partial w_p}\right) 1 \dots r F = 1 \dots r I, \quad (6)$$

where $1 \dots r I = 1 \dots r I(1 \dots r F)$ is a functional of $1 \dots r F$. Such an equation—if it exists—will depend on the studied "gas" and the considered physical conditions. However, with the help of realistic hypotheses, it is theoretically possible to supply an approximate expression with approximations over BY r . However, one must be able to fix the adapted r rank beforehand.

IV. SYSTEMS OF THE EQUATIONS OF MOMENTS EQUIVALENT TO BY r AND ME r

The moments $1 \dots r M_{\rho_1 \dots \rho_l}(x_\rho, t)$ of the distribution function $1 \dots r F(x_\rho, w_\rho, t)$, have by definition the expression

$$1 \dots r M_{\rho_1 \dots \rho_l} = \int \underline{d^{1 \dots r}w} 1 \dots r F w_{\rho_1 \dots \rho_l}, \quad l=0, 1, \dots, +\infty. \quad (7)$$

We will also use an expression including (7) on defining the "projected moments" which we will subsequently call "projection":

$$1 \dots r \dots u M_{\rho_1 \dots \rho_l} = \int \underline{d^{1 \dots r}w} 1 \dots r \dots u F w_{\rho_1 \dots \rho_l}, \quad l=0, 1, \dots, +\infty, \quad (8)$$

$1 \dots r \dots u M_{\rho_1 \dots \rho_l}(x_\rho, t, x_{r+1}, \dots, x_u, w_{r+1}, \dots, w_u)$ is the "projected moment" of $1 \dots r \dots u F$ by $1 \dots r F$ by $1 \dots r F$.

With the aim of obtaining a system equivalent to BY r , let us make the operator $\int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l}$ act on (5). We obtain respectively the terms

$$\int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} \frac{\partial}{\partial t} 1 \dots r F = \frac{\partial}{\partial t} 1 \dots r M_{\rho_1 \dots \rho_l}, \quad (9)$$

$$\int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} w_{\rho_{l+1}} \frac{\partial}{\partial x_{\rho_{l+1}}} 1 \dots r F = \frac{\partial}{\partial x_{\rho_{l+1}}} 1 \dots r M_{\rho_1 \dots \rho_l \rho_{l+1}}. \quad (10)$$

The two following terms require more detail; the third is transformed by integrating by parts,

$$\begin{aligned} & \int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} w_{\rho_{l+1}} a_{\rho_{l+1}}^{1 \dots r} \frac{\partial}{\partial w_{\rho_{l+1}}} 1 \dots r F \\ &= - a_{\rho_{l+1}}^{1 \dots r} \int \underline{d^{1 \dots r}w} \frac{\partial (w_{\rho_1 \dots \rho_l} w_{\rho_{l+1}})}{\partial w_{\rho_{l+1}}} 1 \dots r F \\ &= - a_{\rho_{l+1}}^{1 \dots r} \int \underline{d^{1 \dots r}w} 1 \dots r F \delta_{\rho_{l+1} \langle \rho_l} w_{\rho_1 \dots \rho_{l-1}} \\ &= - a_{\rho_l}^{1 \dots r} \int \underline{d^{1 \dots r}w} 1 \dots r F w_{\rho_1 \dots \rho_{l-1}} \\ &= - a_{\rho_l}^{1 \dots r} M_{\rho_1 \dots \rho_{l-1}}. \end{aligned} \quad (11)$$

Lastly, the fourth term, called the "collisional term," is written

$$\begin{aligned} & \int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} \int \underline{d^{r+1}x} \underline{d^{r+1}w} a_{\rho_{l+1}}^{r+1} \frac{\partial}{\partial w_{\rho_{l+1}}} 1 \dots r+1 F \\ &= \int \underline{d^{r+1}x} \underline{d^{r+1}w} a_{\rho_{l+1}}^{r+1} \int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} \frac{\partial 1 \dots r+1 F}{\partial w_{\rho_{l+1}}} \\ &= - \int \underline{d^{r+1}x} \underline{d^{r+1}w} a_{\rho_{l+1}}^{r+1} \int \underline{d^{1 \dots r}w} 1 \dots r+1 F \frac{\partial (w_{\rho_1 \dots \rho_l})}{\partial w_{\rho_{l+1}}} \\ &= - \int \underline{d^{r+1}x} a_{\rho_{l+1}}^{r+1} \int \underline{d^{1 \dots r+1}w} 1 \dots r+1 F \delta_{\rho_{l+1} \langle \rho_l} w_{\rho_1 \dots \rho_{l-1}} \\ &= - \int \underline{d^{r+1}x} a_{\rho_l}^{r+1} 1 \dots r+1 M_{\rho_1 \dots \rho_{l-1}}. \end{aligned} \quad (12)$$

The sum of the terms (9), (10), (11), and (12) constitutes the system of the equations of moments equivalent to BY r and we obtain:

$$\begin{aligned} \frac{\partial}{\partial t} 1 \dots r M_{\rho_1 \dots \rho_l} + \frac{\partial}{\partial x_{\rho_{l+1}}} 1 \dots r M_{\rho_1 \dots \rho_{l+1}} &= a_{\rho_l}^{1 \dots r} 1 \dots r M_{\rho_1 \dots \rho_{l-1}} \\ &+ \int \underline{d^{r+1}x} a_{\rho_l}^{r+1} 1 \dots r+1 M_{\rho_1 \dots \rho_{l-1}}, \end{aligned} \quad (13)$$

$$r=1, 2, \dots, N-1, \quad l=0, 1, \dots, +\infty.$$

An important case is the one obtained on making $l=0$ in (13),

$$\frac{\partial}{\partial t} 1 \dots r M + \frac{\partial}{\partial x_\rho} 1 \dots r M_\rho = 0. \quad (14)$$

This equation, expressing the conservation of the r -plet, is a generalization of the equation for the conservation of the particles. It will constitute one of the first selection criteria for choosing a master equation.

Likewise, on applying the operator $\int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l}$ on (6), we obtain the set of equations:

$$\begin{aligned} \frac{\partial}{\partial t} 1 \dots r M_{\rho_1 \dots \rho_l} + \frac{\partial}{\partial x_{\rho_{l+1}}} 1 \dots r M_{\rho_1 \dots \rho_{l+1}} \\ = a_{\rho_l}^{1 \dots r} 1 \dots r M_{\rho_1 \dots \rho_{l-1}} + 1 \dots r J_{\rho_1 \dots \rho_l} \end{aligned} \quad (15)$$

$$r=1, \dots, N-1, \quad l=0, 1, \dots, +\infty,$$

where

$$1 \dots r J_{\rho_1 \dots \rho_l} = \int \underline{d^{1 \dots r}w} w_{\rho_1 \dots \rho_l} 1 \dots r I.$$

Expressions (15) constitute the equations of moments equivalent to the master equations (6). A "gas," whose behavior is approached by kinetic theory, may indifferently be shown by (6) or by (15) according to the required applications or uses. In particular, if the par-

ticles are conserved, one must have ${}^{1\cdots r}I$ such that

$${}^{1\cdots r}J = \int d^{1\cdots r}w \quad {}^{1\cdots r}I = 0.$$

V. EQUATIONS OF "HYDRODYNAMIC" QUANTITIES

If the physical conditions are adapted to a hydrodynamic approach, it is useful to define the first "hydrodynamic" quantities from (7) and (8). To do this, we will call density r -tuple the first moment of ${}^{1\cdots r}F$ and will symbolize it by ${}^{1\cdots r}n = {}^{1\cdots r}M$.

In the same way and by analogy to the first rank, we define the average velocity r -tuple ${}^{1\cdots r}v_p$ by using the second moment of ${}^{1\cdots r}F$,

$${}^{1\cdots r}n \quad {}^{1\cdots r}v_p = {}^{1\cdots r}M_p.$$

The mass of the particle being m , we are able to define the hydrodynamic quantity of the l th order of rank r ,

$${}^{1\cdots r}p_{\rho_1 \dots \rho_l} = m^{(r)} \int d^{1\cdots r}w (w_{\rho_1} - {}^{1\cdots r}v_{\rho_1}) \dots (w_{\rho_l} - {}^{1\cdots r}v_{\rho_l}) {}^{1\cdots r}F. \quad (16)$$

In particular, we have for the terms of the first orders:

$${}^{1\cdots r}p = m^{(r)} \quad {}^{1\cdots r}n,$$

$${}^{1\cdots r}p_{\rho_1} = 0,$$

$${}^{1\cdots r}p_{\rho_1 \rho_2} = m^{(r)} ({}^{1\cdots r}M_{\rho_1 \rho_2} - {}^{1\cdots r}n \quad {}^{1\cdots r}v_{\rho_1} \quad {}^{1\cdots r}v_{\rho_2}), \quad (17)$$

$${}^{1\cdots r}p_{\rho_1 \rho_2 \rho_3} = m^{(r)} ({}^{1\cdots r}M_{\rho_1 \rho_2 \rho_3} + 2 \quad {}^{1\cdots r}n \quad {}^{1\cdots r}v_{\rho_1} \quad {}^{1\cdots r}v_{\rho_2} \quad {}^{1\cdots r}v_{\rho_3} - {}^{1\cdots r}M_{\langle \rho_1 \rho_2} \quad {}^{1\cdots r}v_{\rho_3} \rangle).$$

With the aim of obtaining the equations governing the "hydrodynamic" quantities, relation (17) allows us to write:

$${}^{1\cdots r}M = {}^{1\cdots r}n,$$

$${}^{1\cdots r}M_{\rho_1} = {}^{1\cdots r}n \quad {}^{1\cdots r}v_{\rho_1},$$

$${}^{1\cdots r}M_{\rho_1 \rho_2} = m^{(r)} ({}^{1\cdots r}p_{\rho_1 \rho_2} + {}^{1\cdots r}n \quad {}^{1\cdots r}v_{\rho_1} \quad {}^{1\cdots r}v_{\rho_2}), \quad (18)$$

$${}^{1\cdots r}M_{\rho_1 \rho_2 \rho_3} = m^{(r)} ({}^{1\cdots r}p_{\rho_1 \rho_2 \rho_3} + {}^{1\cdots r}p_{\langle \rho_1 \rho_2} \quad {}^{1\cdots r}v_{\rho_3} \rangle + {}^{1\cdots r}n \quad {}^{1\cdots r}v_{\rho_1} \quad {}^{1\cdots r}v_{\rho_2} \quad {}^{1\cdots r}v_{\rho_3}).$$

To lighten the notation to the extent where the rank r is fixed, we henceforth set:

$$n = {}^{1\cdots r}n, \quad v_p = {}^{1\cdots r}v_p, \quad p_{\rho_1 \dots \rho_l} = {}^{1\cdots r}p_{\rho_1 \dots \rho_l},$$

$$a_p = a_p^{1\cdots r}, \quad J_{\rho_1 \dots \rho_l} = {}^{1\cdots r}J_{\rho_1 \dots \rho_l}.$$

On taking account of relation (18) and on combining the equations of moments (15) relative to a master equation of rank r , we obtain the set of hydrodynamic generalized equations:

$$\frac{\partial}{\partial t} n + \frac{\partial}{\partial x_{\rho_1}} (n v_{\rho_1}) = J,$$

$$n m^{(r)} \frac{\partial}{\partial t} v_{\rho_1} + v_{\rho_2} \frac{\partial}{\partial x_{\rho_2}} v_{\rho_1} + \frac{\partial}{\partial x_{\rho_2}} p_{\rho_1 \rho_2} = m^{(r)} (J_{\rho_1} + a_{\rho_1} n v_{\rho_1} J),$$

$$\frac{\partial}{\partial t} p_{\rho_1 \rho_2} + \frac{\partial}{\partial x_{\rho_3}} (p_{\rho_1 \rho_2 \rho_3} + v_{\rho_3} p_{\rho_1 \rho_2}) + p_{\rho_3 \langle \rho_1} \frac{\partial v_{\rho_2} \rangle}{\partial x_{\rho_3}} = m^{(r)} (J_{\rho_1 \rho_2} - v_{\rho_1} J_{\rho_2} + v_{\rho_1 \rho_2} J). \quad (19)$$

It is interesting to note that these equations are formally identical to the classical equations of hydrodynamics; the latter, moreover, are obtained as particular cases when, in (19), we set $r=1$; the distinction is only made with the possible values of the signs ρ which allow the fixing of the rank r . The detail of Eqs. (19) passes by the knowledge of the corresponding master equation which allows us to calculate the J .

VI. CONCLUSIONS

The immediate exploitation of Eqs. (13) and (19) is not possible. However, their existence, like that of the BBGKY system, allows the physicist to have a base upon which he will "graft" his approximations in order to obtain a useful model for the applications.

For example, if a master equation [of type (6)] correctly shows the behavior of a population of N particles, one may, if necessary, use a method comparable to that developed by Grad with Boltzmann's equation if the macroscopic behavior is "fluid." That is to say that in the right-hand sides of (19) (the integral terms), one uses an approximation of ${}^{1\cdots r}F$ on curtailing the infinite series,

$${}^{1\cdots r}F = \frac{\exp(-w^2/2)}{(2\pi)^{3r/2}} \sum_{l=0}^{\infty} \frac{1}{l!} \quad {}^{1\cdots r}C_{\rho_1 \dots \rho_l}(t, x_p) \quad {}^{1\cdots r}H_{\rho_1 \dots \rho_l}(u_p), \quad (20)$$

knowing that, to define $\overline{{}^{1\cdots r}F}$, one sets

$${}^{1\cdots r}F = \left\{ \prod_{i=1}^r n \left(\frac{m}{k^T T} \right)^{3/2} \right\} \quad {}^{1\cdots r}\psi \quad \overline{{}^{1\cdots r}F}, \quad (21)$$

${}^{1\cdots r}H_{\rho_1 \dots \rho_l}$ are the Hermite tensorial polynomials,¹⁰ and ${}^{1\cdots r}\psi$ is the correlation function.

One easily shows from (20) that the coefficients C are written

$${}^{1\cdots r}C_{\rho_1 \dots \rho_l}(t, x_p) = \int d^{1\cdots r}w \quad {}^{1\cdots r}H_{\rho_1 \dots \rho_l} \quad \overline{{}^{1\cdots r}F}. \quad (22)$$

It seems that this work finds applications in the calculations of the fluid transport coefficients when Boltzmann's equation or any other kinetic equation (of order 1) fails—quite obviously—to the extent that a representative master equation exists.

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Scalar-vector instantons in n dimensions: Surface terms

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By an analysis that respects surface terms, it is shown that the equations of motion for a non-Abelian gauge field A_μ^a coupled to a scalar field Φ^i possess no regular, finite-action solutions in n -dimensional Euclidean space except for $n = 4$, with Φ trivial, and for $n < 4$.

It has been known for about a year that the equations of motion for a non-Abelian gauge field A_μ^a coupled to a scalar field Φ^i have no regular¹, finite-action solutions in n -dimensional Euclidean space except for $n = 4$, with Φ trivial, and for $n < 4$. Most proofs² of this result seem, however, to assume the absence of certain surface terms. The purpose of the present note is to provide a demonstration that is independent of that assumption.

The action functional S will be taken as the integral $\int d^n x \mathcal{L}(x)$ of the Lagrange density

$$\mathcal{L}(x) = \frac{1}{4} F_{\mu\nu}^a(x)^2 + \frac{1}{2} |D_\mu^i \Phi(x)|^2 + V[\Phi^i(x)],$$

where

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a - ef_{abc} A_\mu^b A_\nu^c$$

and

$$D_\mu^i \Phi = \partial_\mu \Phi^i + ie A_\mu^a t_{ij}^a \Phi^j.$$

The matrices t^a are the hermitian generators of a representation g of a compact Lie group G whose structure constants are f_{abc} . The potential V is assumed to be nonnegative.

Under the Derrick³ transformation, $\Phi(x, \lambda) = \Phi(\lambda x)$ and $A_\mu(x, \lambda) = \lambda A_\mu(\lambda x)$, the action becomes

$$S(\lambda) = \lambda^{4-n} S_A + \lambda^{2-n} S_\Phi + \lambda^{-n} S_V,$$

where S_A , S_Φ , and S_V are the contributions of the vector field A_μ , the scalar field Φ , and the potential V evaluated at $\lambda = 1$. These terms are all positive and finite if the fields A_μ and Φ are nontrivial and of finite action. The derivative of $S(\lambda)$ at $\lambda = 1$

$$S'(1) = (4-n)S_A + (2-n)S_\Phi - nS_V$$

is strictly negative for $n = 4$, unless Φ is trivial, and for $n > 4$.

It will now be shown that this same derivative $S'(1)$ is positive or zero if the fields $A_\mu(x, 1) = A_\mu(x)$ and $\Phi(x, 1) = \Phi(x)$ constitute a twice continuously differentiable, finite-action solution of the field equations. The demonstration uses an interesting property of the radial gauge, $x_\mu A_\mu^a(x) = 0$, whose universality may be proved by an obvious modification of a well-known argument.⁴ The derivatives of the fields $A_\mu(x, \lambda)$ and $\Phi(x, \lambda)$ with respect to λ at $\lambda = 1$ are

$$\Phi'^i(x, 1) = x_\nu \partial_\nu \Phi^i(x)$$

and

$$A_\mu'^a(x, 1) = A_\mu^a(x) + x_\nu \partial_\nu A_\mu^a(x).$$

In the radial gauge, these derivatives are

$$\Phi'^i(x, 1) = x_\nu D_\nu^i \Phi(x)$$

and

$$A_\mu'^a(x, 1) = x_\nu F_{\nu\mu}^a(x).$$

Let $S(\lambda, < R)$ denote the action due to the fields $A_\mu(x, \lambda)$ and $\Phi(x, \lambda)$ for $|x| \leq R$. Then from the assumption that the fields $A_\mu(x, 1)$ and $\Phi(x, 1)$ constitute a twice continuously differentiable solution of the field equations and from the compactness of the region $|x| \leq R$, it follows that the derivative of $S(\lambda, < R)$ with respect to λ at $\lambda = 1$ is the integral

$$S'(1, < R) = R^{n-2} \int d\Omega \left[x_\rho F_{\rho\mu}^a A_\mu'^a + \frac{1}{2} (D_\rho^i \Phi)^* \Phi'^i + \frac{1}{2} (\Phi'^i)^* D_\rho^i \Phi \right]$$

over the surface of the sphere $|x| = R$. In the radial gauge, this surface term is

$$S'(1, < R) = R^{n-2} \int d\Omega \left(x_\rho F_{\rho\mu}^a \right)^2 + |x_\rho D_\rho^i \Phi|^2 \geq 0,$$

which cannot be negative.

The action $S(\lambda, > R)$ due to the fields $A_\mu(x, \lambda)$ and $\Phi(x, \lambda)$ for $|x| > R$ consists of three terms that may be written as

$$\begin{aligned} S(\lambda, > R) &= S_A(\lambda, > R) + S_\Phi(\lambda, > R) + S_V(\lambda, > R) \\ &= \lambda^{4-n} S_A(1, > \lambda R) + \lambda^{2-n} S_\Phi(1, > \lambda R) \\ &\quad + \lambda^{-n} S_V(1, > \lambda R) \end{aligned}$$

in an obvious notation. Thus

$$\begin{aligned} S'(1, > R) &= (4-n)S_A(1, > R) + (2-n)S_\Phi(1, > R) \\ &\quad - nS_V(1, > R) + R \partial S(1, > R) / \partial R. \end{aligned}$$

If the action of the hypothetical solution $A_\mu(x, 1)$ and $\Phi(x, 1)$ is finite, then the first three terms on the right-hand side of this equation can be made arbitrarily small by increasing R sufficiently. Similarly, there must be a sequence of points R_i , tending to infinity, on which the product $R_i \partial S(1, > R_i) / \partial R$ tends to zero; for otherwise the action would be at least logarithmically divergent. Thus, since

$$S'(1) = S'(1, < R_i) + S'(1, > R_i) \geq S'(1, > R_i),$$

it follows that $S'(1) \geq 0$ as promised.

Suppose now that the potential $V(\Phi^a)$ is invariant under the action of the group G , that $\Phi_0 \neq 0$ is one of its minima, and that the homotopy group $\pi_{n-1}(G/H) \neq 0$, where H is the little group of Φ_0 . One may look for the field configuration that has the least action in each homotopy class. The fields

$$\Phi(x) = f(|x|)g(\hat{x})\Phi_0$$

and

$${}^{\mu}A_{\mu}^a(x) = (i/e)h(|x|)\partial_{\mu}g(\hat{x})g^{-1}(\hat{x}),$$

where $\hat{x} = x/|x|$ will have finite action if f and h are smooth functions that rise (h like x^2) from zero at $x=0$ to one at $|x|=r$ and that remain equal to one for $|x|>r$. A very crude estimate of the action of such a configuration is

$$S_A \approx e^{-2}r^{n-4}, \quad S_{\Phi} \approx r^{n-2}, \quad \text{and} \quad S_V \approx r^n.$$

Thus, for $n > 4$, the singular configurations with $r=0$ all have minimal action, $S=0$. Also for $n=4$, and Φ nontrivial, the singular configurations with $r=0$ have minimal action S equal to that of the same system without the scalar field, provided the latter possesses suitable solutions.⁵ For $n < 4$, the least action is that of

the solution to the field equations, whenever the latter exists.

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¹By regular is meant twice continuously differentiable. The solutions of elliptic partial-differential equations are typically analytic, so this assumption is not unduly restrictive. See, e.g., C. Miranda, *Partial Differential Equations of Elliptic Type* (Springer-Verlag, Berlin, 1970), pp. 214–15.

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Killing vectors in plane HH spaces

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Employing the spinorial approach to the structure of hyperheavens, we integrate completely the Killing vector equations for plane (case I) hyperheavens, reducing them to one master equation of an extremely plausible form. (In this process, optimally simple gauges are demonstrated for each Petrov type.) The mechanism of generating Ernst potentials by Killing vectors is then investigated, and explicit forms are given. Also, some interesting preliminary study of Killing spinors of type $D(0,k)$ in heavens is presented.

1. INTRODUCTION

This is a paper in the series on the structure of hyperheavens (HH spaces)—left-degenerate solutions of the complex Einstein equations, in vacuum or with the cosmological constant or an electromagnetic field properly aligned with the complex gravity—initiated by Plebański and Robinson.¹ The principal reason for our interest in these solutions is that their real slices describe, among other things, *all* algebraically degenerate *real-valued* solutions of the vacuum Einstein equations. It is therefore of interest to investigate the roots of the possible symmetries of these real solutions, still on the level of the complex-valued theory, where general regularities are more easily noticed and effectively treated. Moreover, we know² that in the case of (complex) heavenly manifolds— H spaces—all the Killing equations can be effectively integrated, reducing problems of determinations of symmetries to the study of one single master equation.

In this paper we restrict ourselves to the case of plane hyperheavens (those with zero expansion, called case I in Ref. 1), and show that the earlier work on Killing vectors in heavens² can be extended to these plane hyperheavens (and, therefore, to certain real spacetimes). The spinorial techniques introduced by Boyer and Plebański³ and developed by Finley and Plebański⁴ are used throughout since they permit considerable simplifications for the effective integration of the equations, relative to the techniques used in heavens.²

To illustrate this, we also include the *spinorial* derivation of the master Killing equation for heavens in the present condensed notation, as a special case of the more general problem considered here. Working with these spinorial techniques, however, it is most useful to examine carefully the role of the group of automorphisms of the tetrad (and therefore the metric) in the description of the results derived. We will point out here in detail how this group, first

mentioned in Ref. 1, can be used to simplify greatly the constraints on the parameters involved in the final equations, depending upon the specific (complex) Petrov type in question.

We recall that the existence of a Killing (vector) structure in a space allows one to formulate a (complex) Ernst potential⁵ which may be used as a means not only of describing the geometric structures of the space itself, but also as a starting point for certain generalizations to more complicated spaces as well.⁶ Since, by our technique, Killing's equations have been essentially integrated, we can also give an explicit form for the associated Ernst potentials for our plane HH spaces, which may then be used as starting points for such generalizations. While executing this program, we also noticed that the equations for general Killing spinors⁷ of type $D(0,k)$ possess highly interesting properties. It turns out that a ladder of key functions (and corresponding spinorial coordinates) for heavens introduced in Ref. 3 becomes essential in the treatment of these spinors. (It seems very likely that a similar such ladder exists in general HH spaces.)

2. THE MASTER KILLING VECTOR EQUATION

We are concerned with Killing vectors as well as Killing spinors, all in a coordinate system adapted to a spinorial form. It is therefore most convenient to look at the equations that determine a (conformal) Killing vector [$K_{(\mu;\nu)} = \chi g_{\mu\nu}$] in a spinorial formalism. We denote the Killing 1-form by an (equivalent) $D(\frac{1}{2}, \frac{1}{2})$ spinor,

$$K = -\frac{1}{2} g^{A\dot{B}} K_{A\dot{B}}, \quad (2.1)$$

where $g^{A\dot{B}}$ is the usual mapping from 1-form to $D(\frac{1}{2}, \frac{1}{2})$ spinors.⁸ Killing's equations may then be written as the nine equations

$$E_{RS}{}^{\dot{A}\dot{B}} \equiv \nabla_{(R} (\dot{A} K_{S)}^{\dot{B}}) = 0, \quad (2.2)$$

which imply⁷ the existence of symmetric spinors $\ell_{\dot{A}\dot{B}}$ and ℓ_{RS} such that

$$\nabla_R{}^{\dot{A}K_S{}^{\dot{B}}} = \ell_{RS} \epsilon^{\dot{A}\dot{B}} + \ell^{\dot{A}\dot{B}} \epsilon_{RS} - 2\epsilon_{RS} \epsilon^{\dot{A}\dot{B}} \chi, \quad (2.3a)$$

where

$$\ell_{RS} = \frac{1}{2} \epsilon^{\dot{A}\dot{B}} \nabla_{(R} (\dot{A} K_{S)}^{\dot{B}}), \quad \ell^{\dot{A}\dot{B}} = \frac{1}{2} \epsilon^{RS} \nabla_R (\dot{A} K_S^{\dot{B}}), \quad (2.3b)$$

while $\nabla_R{}^{\dot{A}} = g_R{}^{\dot{A}\mu} \nabla_\mu$ are just the spinorial components of

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the covariant derivative, and

$$\chi = -\frac{1}{6}\epsilon_{\dot{A}\dot{B}\dot{C}}{}^{RS}\nabla_R\dot{A}K_S{}^{\dot{B}} \quad (2.3c)$$

is the same as in the vectorial version.

It is shown in Ref. 7 (see also Ref. 12) that the integrability conditions for these equations, in a Ricci-flat space such as we consider here, may be written as

$$L_{RST}{}^{\dot{A}} = \nabla_R{}^{\dot{A}}\ell_{ST} + 2K_U{}^{\dot{A}C}{}_{RST} = 0, \quad (2.4a)$$

$$M_{RSTU} \equiv K_{PA}{}^{\dot{A}}\nabla^P C_{RSTU} - 4\chi C_{RSTU} + 4\ell_{V(R}C^V{}_{STU)} = 0, \quad (2.4b)$$

and similar equations for the objects with dotted indices. (We have also assumed χ to be constant, thus actually restricting our discussion to homothetic Killing vectors because it is well known^{2,7} that otherwise we can only pursue studies of spaces which are of type $[N] \otimes [N]$ or more conformally flat.)

We recall that, in the tetrad and coordinates of Ref. 4, the metric for a plane hyperheaven is determined by spinor coordinates $p^{\dot{A}}q_{\dot{B}}$, a key function Θ , and two auxiliary functions $F^{\dot{C}}$ and $N^{\dot{D}}$, constant on each null string—i. e., functions of $q_{\dot{B}}$ only—such that

$$\begin{aligned} ds^2 &= 2E^{\dot{A}}{}_{\dot{B}} e_{\dot{A}} e_{\dot{B}}, \quad E^{\dot{A}}{}_{\dot{B}} = -dq^{\dot{A}} + Q^{\dot{A}\dot{B}}dq_{\dot{B}} + (2)^{-1/2}g^{\dot{A}\dot{B}}, \\ e_{\dot{A}} &= dq_{\dot{A}} - (2)^{-1/2}g_{\dot{A}\dot{B}}, \quad Q^{\dot{A}\dot{B}} = -\partial^{\dot{A}}\partial^{\dot{B}}\Theta + \frac{2}{3}F^{\dot{A}}p^{\dot{B}}, \end{aligned} \quad (2.5)$$

where Θ must satisfy the (plane) hyperheavenly equation³:

$$\begin{aligned} \frac{1}{2}(\partial^{\dot{A}}\partial^{\dot{B}}\Theta)\partial_{\dot{A}}\partial_{\dot{B}}\Theta + \partial^{\dot{A}}\Theta_{,\dot{A}} + F^{\dot{A}}\partial_{\dot{A}}\Theta - \frac{2}{3}F^{\dot{A}}p^{\dot{B}}\partial_{\dot{A}}\partial_{\dot{B}}\Theta \\ + (F^{\dot{A}}p_{\dot{A}})^2/18 + \frac{1}{6}p^{\dot{A}}p^{\dot{B}}F_{\dot{A}\dot{B}} + N^{\dot{A}}p_{\dot{A}} = 0, \end{aligned} \quad (2.6a)$$

which implies the existence of a potential Λ such that

$$\begin{aligned} \partial_{\dot{A}}\Lambda = 2\Theta_{,\dot{A}} + (\partial_{\dot{A}}\partial_{\dot{B}}\Theta)\partial^{\dot{B}}\Theta + \frac{10}{3}F_{\dot{A}}\Theta - \frac{4}{3}F_{\dot{A}}p_{\dot{B}}\partial^{\dot{B}}\Theta \\ + (F^{\dot{B}}p_{\dot{B}})^2p_{\dot{A}}/36 + F_{\dot{B}\dot{C}}p^{\dot{B}}p^{\dot{C}}p_{\dot{A}}/12 + \frac{2}{3}N^{\dot{B}}p_{\dot{B}}p_{\dot{A}}. \end{aligned} \quad (2.6b)$$

We will also need the (spinorial) expressions for the connections and the components of the conformal curvature tensor:

$$\begin{aligned} \Gamma_{11} = 0, \quad \Gamma_{12} = \frac{1}{2}F^{\dot{A}}e_{\dot{A}}, \quad \Gamma_{22} = (N^{\dot{A}} + \frac{1}{2}p^{\dot{A}}F^{\dot{B}}{}_{,\dot{B}})e_{\dot{A}} \equiv V^{\dot{A}}e_{\dot{A}}, \\ \Gamma_{\dot{A}\dot{B}} = -(\partial_{\dot{A}}\partial_{\dot{B}}\partial_{\dot{C}}\Theta)e^{\dot{C}} + \frac{1}{3}F_{\dot{A}\dot{B}}e^{\dot{C}}, \quad (2.7) \\ C_{\dot{A}\dot{B}\dot{C}\dot{D}} = \partial_{\dot{A}}\partial_{\dot{B}}\partial_{\dot{C}}\partial_{\dot{D}}\Theta, \\ C_{1111} = 0 = C_{1112} = C_{1122}, \quad C_{1222} = -\frac{1}{2}F^{\dot{A}}{}_{,\dot{B}}, \\ C_{2222} = \left(F^{\dot{A}} - \frac{\partial}{\partial q_{\dot{A}}}\right)V_{\dot{A}}, \end{aligned}$$

where $\partial_{\dot{A}} = \partial/\partial p^{\dot{A}}$ and $H^{\dot{A}} \equiv \partial H/\partial q_{\dot{A}}$. (notice also that $\partial_{\dot{A}}$ and $\delta^{\dot{A}} \equiv \partial/\partial q_{\dot{A}} + Q^{\dot{A}\dot{B}}\partial_{\dot{B}}$ form a dual basis for the tangent space.) We also commonly write $\Gamma_{AB} \equiv \Gamma_{AB\dot{C}}e^{\dot{C}}$. In the case where $F^{\dot{A}}$ and $N^{\dot{A}}$ may be chosen to vanish, this becomes a heavenly space (left-flat).

Having given enough notation and background to be able to proceed, we will now state the results which specify when a given plane hyperheaven will admit any (homothetic) Killing vectors, and then exhibit explicitly the Ernst potentials associated with any allowed ordinary Killing vector ($\chi_0 = 0$). We will give the complete derivation in the following section.

We find that a plane hyperheaven admits a Killing vector, K , if and only if the key function Θ , which generates the metric, satisfies the following plausible equation for its Lie derivative,

$$\mathcal{L}_K\Theta = 2\omega\Theta - 2\alpha_0\Lambda + P, \quad (2.8)$$

where P is a third-order polynomial in the $p^{\dot{A}}$ variables with coefficients which are arbitrary functions of $q_{\dot{B}}$,

$$P \equiv \frac{1}{6}\delta_{\dot{A}\dot{B}\dot{C}}{}^{\dot{D}}\dot{C}p^{\dot{A}}p^{\dot{B}}p^{\dot{C}} + (\frac{1}{2}\epsilon_{\dot{A}\dot{B}}{}^{\dot{C}} + \frac{1}{3}F_{\dot{A}\dot{B}})p^{\dot{A}}p^{\dot{B}} + \zeta^{\dot{A}}p_{\dot{A}} + \eta, \quad (2.9)$$

while α_0 is a constant which vanishes unless the space is left-flat, Λ is a prolongation of Θ satisfying Eq. (2.6) which is only needed for left-flat spaces, while $\omega = 3\chi_0 - \delta^{\dot{A}}{}_{,\dot{A}}$ (with χ_0 constant) is a function of $q_{\dot{B}}$ only which may always be chosen to be a constant by proper choice of gauge in any particular type of space. In this form, the Killing vector in question is determined by α_0 , χ_0 , and the coefficients of P by the following equation (written in a coordinate basis for reasons of simplicity of form):

$$K = (\alpha_0 p_{\dot{A}} + \delta_{\dot{A}})\frac{\partial}{\partial q_{\dot{A}}} + (2\alpha_0\partial^{\dot{A}}\Theta + \delta^{\dot{B}}{}_{,\dot{A}}p_{\dot{B}} + 2\chi_0 p^{\dot{A}} + \epsilon^{\dot{A}})\partial_{\dot{A}}. \quad (2.10)$$

We refer to Eq. (2.8), with Eq. (2.9) inserted for P and Eq. (2.10) inserted for K , as the *master Killing vector equation*, which gives the explicit requirements that a metric (for a plane HH space) must satisfy to admit a symmetry generated by a Killing vector. This equation then serves as a much simpler way to convey the same information as the complete set of usual Killing equations: 10 first-order partial differential equations for four unknown functions of four independent variables. This single compatibility equation can be used to generate metrics with desired symmetries, or the symmetries of a given metric. In general, there are as many solutions for a Killing vector as there are independent sets of functions α_0 , χ_0 , $\delta_{\dot{A}}$, and $\epsilon^{\dot{B}}$ which satisfy the master equation.

Explicit constraints on $\delta_{\dot{A}}$, $\epsilon^{\dot{A}}$, and $\zeta_{\dot{A}}$ are created by the integrability conditions [Eqs. (2.4)] of the original set. The general form of these equations will be given in Sec. 3; we give here only the forms simplified according to the (complex) Petrov type in question. In the case [III] \otimes [anything], we may so choose the gauge (see Sec. 3) that $F^{\dot{A}} = \frac{1}{2}q^{\dot{A}}$, $N^{\dot{A}} = 0$, and we have

$$\delta^{\dot{A}} = b'{}^{\dot{A}}, \quad q^{\dot{A}}b_{,\dot{A}} = 2b, \quad \alpha_0 = 0, \quad (2.11a)$$

$$\epsilon^{\dot{A}} = a'{}^{\dot{A}} - \frac{1}{2}aq^{\dot{A}}, \quad q^{\dot{A}}a_{,\dot{A}} = -4a, \quad 2\zeta^{\dot{B}}{}_{,\dot{B}} = q^{\dot{B}}\zeta_{\dot{B}},$$

where a and b must therefore be arbitrary homogeneous functions (of the variables $q_{\dot{A}}$) of order $+2$ and -4 , respectively.¹⁰ In the case $[N] \otimes$ [anything], we may so choose the gauge that $F^{\dot{A}} = 0$, and we then obtain

$$\begin{aligned} \delta^{\dot{A}} &= [(2\chi_0 - \rho_0)N^{\dot{A}} + \xi^{\dot{A}}]/N^{\dot{B}}{}_{,\dot{B}}, \\ \delta^{\dot{A}}{}_{,\dot{A}} &= \rho_0 = -b, \quad \alpha_0 = 0, \\ \epsilon^{\dot{A}}{}_{,\dot{A}} &= -2(\xi - N^{\dot{A}}\xi_{,\dot{A}}/N^{\dot{B}}{}_{,\dot{B}}), \quad \zeta^{\dot{B}}{}_{,\dot{B}} = \epsilon^{\dot{B}}N_{\dot{B}}, \end{aligned} \quad (2.11b)$$

where ξ is an arbitrary function of $q_{\dot{B}}$ only. Finally, in the case $[-] \otimes$ [anything]—left-flat—we may choose

$N^{\dot{A}} = 0 = F^{\dot{A}}$ and we have

$$\delta^{\dot{A}} = \frac{1}{2}\rho_0 q^{\dot{A}} + \varphi^{\dot{A}}, \quad \epsilon^{\dot{A}} = -\frac{1}{2}\gamma_0 q^{\dot{A}} + \sigma^{\dot{A}}, \quad \zeta^{\dot{A}} = \psi^{\dot{A}}, \quad (2.11c)$$

where γ_0 is a new constant, and φ , σ , and ψ are arbitrary functions of $q_{\dot{A}}$.

Given an ordinary Killing vector we may then formulate an Ernst potential which is a very useful object, not only as a potential for the description of the given geometry, but especially as a tool to use the transformations of the Kinnersley group⁶ to discover generalizations of these plane hyperheavens. Reserving the proofs for Sec. 3, we may here say that for plane hyperheavens which are *not* left-flat, the most general Ernst potentials are of the form

$$\frac{1}{2}\bar{\mathcal{E}} = b\delta_{\dot{B}}p^{\dot{B}} + \nu, \quad \frac{1}{2}\bar{\mathcal{C}} = 2\delta_{\dot{A}}\partial^{\dot{A}}T - \nu, \quad (2.12a)$$

$$\nu^{\dot{A}} = \delta^{\dot{A}}(2N^{\dot{C}}\delta_{\dot{C}} - \epsilon^{\dot{C}}_{\dot{C}}) - b\epsilon^{\dot{A}}, \quad \alpha_0 = 0,$$

while if the space is left-flat, α_0 need not be zero and we have

$$\frac{1}{2}\bar{\mathcal{E}} = 2\alpha_0 T - \rho_0 \delta_{\dot{A}} p^{\dot{A}} + \tau, \quad (2.12b)$$

$$\frac{1}{2}\bar{\mathcal{C}} = 2(\alpha_0 p^{\dot{A}} + \delta_{\dot{A}})\partial^{\dot{A}}T - 2\alpha_0 T - \tau,$$

$$\tau = \gamma_0 \varphi + \rho_0 \sigma + 2\alpha_0 \psi,$$

where the indicated ν and τ are functions of $q_{\dot{A}}$ only, and in both cases

$$T = [\alpha_0(p^{\dot{A}}\partial^{\dot{A}} - 3) + \delta_{\dot{A}}\partial^{\dot{A}}]\Theta + \frac{1}{2}(\delta^{\dot{A},\dot{B}} + \frac{1}{3}\delta^{\dot{A}}F^{\dot{B}})p^{\dot{A}}p^{\dot{B}} + \epsilon^{\dot{A}}p^{\dot{A}}. \quad (2.13)$$

3. DERIVATION OF THE MASTER EQUATION

To solve the equation $E_{RS}^{\dot{A}\dot{B}}$ [Eqs. (2.2)], we first write

$$K = k_{\dot{B}}E^{\dot{B}} + K^{\dot{B}}e_{\dot{B}}, \quad (3.1)$$

and easily calculate that

$$\ell_{11} = \partial_{\dot{A}}k^{\dot{A}}, \quad 2\ell_{12} = \partial_{\dot{A}}K^{\dot{A}} + \partial_{\dot{A}}k^{\dot{A}} + F^{\dot{A}}k_{\dot{A}}, \quad (3.2)$$

$$\ell_{22} = \partial_{\dot{A}}K^{\dot{A}} + V^{\dot{A}}k_{\dot{A}}, \quad 4\chi_0 = \partial_{\dot{A}}k^{\dot{A}} - \partial_{\dot{A}}K^{\dot{A}} + F^{\dot{A}}k_{\dot{A}}.$$

It is simplest to start as high up the ladder of integrability conditions as possible. Using Eqs. (2.4) we find that equations M_{1111} and M_{1112} are trivially satisfied but that M_{1122} and M_{1222} tell us

$$\ell_{11}C^{(2)} = 0, \quad \ell_{11}C^{(1)} + 2\partial_{\dot{A}}(k^{\dot{A}}C^{(2)}) = 0, \quad (3.3)$$

Therefore, $\ell_{11} \neq 0$ only when $C^{(1)}$ and $C^{(2)}$ vanish—only in a left-flat (vacuum) space. We must therefore split the discussion into two cases. We first assume $\ell_{11} \neq 0$. Since the space is left-flat, we may choose a tetrad so that $\Gamma_{AB} = 0$; i. e., $F^{\dot{A}} = 0 = N^{\dot{A}}$. Then the equations $L_{RST}^{\dot{A}}$ just say that l_{RS} must be constant. In this notation, we have

$$E_{11}^{\dot{A}\dot{B}} = \partial^{\dot{A}}k^{\dot{B}} = 0, \quad \ell_{11} = 2\sigma_0 = \partial_{\dot{A}}k^{\dot{A}}, \quad (3.4)$$

which says that

$$k_{\dot{A}} = -\alpha_0 p_{\dot{A}} + \delta_{\dot{A}}, \quad (3.5)$$

where $\delta_{\dot{A}}$ is a function of $q_{\dot{B}}$ only. Then

$$\ell_{12} = \frac{1}{2}\partial_{\dot{A}}K^{\dot{A}} + \frac{1}{2}k^{\dot{A}}_{,\dot{A}} = k^{\dot{A}}_{,\dot{A}} - 2\chi_0, \quad (3.6)$$

tells us that $k^{\dot{A}}_{,\dot{A}} = \delta^{\dot{A}}_{,\dot{A}}$ must be a constant, ρ_0 , and also implies the existence of a scalar T such that

$$K^{\dot{A}} = -\partial^{\dot{A}}T + (\frac{1}{2}\rho_0 - 2\chi_0)p^{\dot{A}}. \quad (3.7)$$

With these forms for both $k_{\dot{A}}$ and $K^{\dot{A}}$, we find that $E_{12}^{\dot{A}\dot{B}}$ becomes just $\partial^{\dot{A}}\partial^{\dot{B}}$ acting on something, which gives us a form for T ,

$$T = k_{\dot{S}}\partial^{\dot{S}}\Theta - 3\alpha_0\Theta + \frac{1}{2}\varphi^{\dot{R}\dot{S}}p_{\dot{R}}p_{\dot{S}} + \epsilon^{\dot{R}}p_{\dot{R}}, \quad (3.8)$$

where we have written

$$\delta^{\dot{A}} = \frac{1}{2}\rho_0 q^{\dot{A}} + \varphi^{\dot{A}},$$

where $\epsilon^{\dot{A}}$ and φ are arbitrary functions of $q_{\dot{B}}$ only. We may now insert all this into $E_{22}^{\dot{A}\dot{B}}$ which says that

$$-\partial^{\dot{A}}\partial^{\dot{B}}T + (\rho_0 - 4\chi_0)Q^{\dot{A}\dot{B}} + [2\partial_{\dot{S}}T + (\rho_0 - 4\chi_0)p_{\dot{S}}]\partial^{\dot{S}}\partial^{\dot{A}}\partial^{\dot{B}}\Theta = 0.$$

By commuting $\partial^{\dot{A}}$ and $\partial^{\dot{B}}$ we easily cause it to take the form of $\partial^{\dot{A}}\partial^{\dot{B}}\Theta = 0$ and thereby imply the existence of γ_0 and $\zeta^{\dot{A}}$ such that

$$\partial^{\dot{A}}T = (\frac{1}{2}\rho_0 - 2\chi_0)\partial^{\dot{A}}[(p_{\dot{S}}\partial^{\dot{S}} - 3)\Theta] + \frac{1}{2}\gamma_0 p^{\dot{A}} + \zeta^{\dot{A}}, \quad (3.9)$$

where the γ_0 that enters must be a constant since $\ell_{22} = \partial_{\dot{A}}K^{\dot{A}} = \gamma_0$. At this point, we note that $\partial_{\dot{A}}\delta^{\dot{A}} = \delta^{\dot{A}}\partial_{\dot{A}}$, while $\delta_{\dot{A}}\delta^{\dot{A}} = 0$. Using Eqs. (3.8) and (3.9), as appropriate, the first fact tells us that $\epsilon^{\dot{A}}_{,\dot{A}} = -\gamma_0$, while the second says that $\zeta^{\dot{A}}_{,\dot{A}} = 0$. This guarantees that $\epsilon^{\dot{A}}$ and $\zeta^{\dot{A}}$ must have the forms given in Eq. (2.11c). We may then insert Eq. (3.8) into Eq. (3.9). This must be simplified by the elimination of all the terms $(\partial^{\dot{A}}\partial^{\dot{B}}\Theta)\partial^{\dot{C}}\partial_{\dot{B}}\Theta$ which appear. To do this we note that this term is skew-symmetric on the free indices, and obtain, using the heavenly equation (2.6a):

$$(\partial^{\dot{A}}\partial^{\dot{B}}\Theta)\partial^{\dot{C}}\partial_{\dot{B}}\Theta = -\frac{1}{2}\epsilon^{\dot{A}\dot{C}}(\partial^{\dot{B}}\partial^{\dot{B}}\Theta)\partial_{\dot{B}}\partial_{\dot{B}}\Theta = \epsilon^{\dot{A}\dot{C}}\partial^{\dot{B}}\partial_{\dot{B}}\Theta.$$

Also we use Eq. (2.6b) to reduce certain complicated coefficients of α_0 to merely $2\partial_{\dot{A}}\Lambda$. The equation is then rewritten as the vanishing of $\partial^{\dot{A}}$ on something; this implies the existence of η —a function of $q_{\dot{B}}$ only—and gives us the master equation.¹¹

Now in the case that $\alpha_0 = 0$, so that at least one of $C^{(1)}$ or $C^{(2)}$ may be nonzero, we still have that $k_{\dot{A}} = \delta_{\dot{A}}$ [Eq. (3.5) with $\alpha_0 = 0$].

However, Eq. (3.3)— M_{1222} —then insists that $(\delta^{\dot{A}}C^{(2)})_{,\dot{A}} = 0$, or that there is a b such that

$$F^{\dot{B}}_{,\dot{B}}\delta^{\dot{A}} = b^{\dot{A}}. \quad (3.10)$$

Equation $L_{212}^{\dot{A}}$ then becomes $(\ell_{12} + b)^{\dot{A}} = 0$. Insertion of this into the definition of ℓ_{12} and a choice of constant so that $\ell_{12} + b = -2\chi_0$, gives us a first-order equation,

$$-b = \delta^{\dot{A}}_{,\dot{A}} + F^{\dot{A}}\delta_{\dot{A}} = -(F^{\dot{B}}_{,\dot{B}})^{-1}b^{\dot{A}}[F_{\dot{A}} + (F^{\dot{C}}_{,\dot{C}})^{-1}F^{\dot{B}}_{,\dot{B}}] \quad (3.11)$$

which determines it in terms of an arbitrary function of one variable as soon as $F_{\dot{A}}$ is known. When a specific Petrov type is decided we can say more about it.

We also know ℓ_{12} in terms of $\partial_{\dot{A}}K^{\dot{A}}$; in particular, the equation is $-\partial_{\dot{A}}K^{\dot{A}} = b + 4\chi_0$, which gives us

$$K^{\dot{A}} = -\partial^{\dot{A}}T - \frac{1}{2}(b + 4\chi_0)p^{\dot{A}} \quad (3.12)$$

in terms of some scalar function T . Inserting this into $\frac{1}{2}E_{12}^{\dot{A}\dot{B}} = \partial^{\dot{A}}(K^{\dot{B}}) + \delta^{\dot{A}}(K^{\dot{B}}) - k_{\dot{B}}\partial^{\dot{A}}(Q^{\dot{B}})\dot{s}$, it reduces to the form $\partial^{\dot{A}}(U^{\dot{B}}) = 0$, where again $U^{\dot{B}}$ is used as a generic symbol, giving us

$$T = \delta_{\dot{B}}\delta^{\dot{B}}\Theta + \frac{1}{2}(\delta^{\dot{A}}\dot{s} + \frac{1}{3}\delta^{\dot{R}}F^{\dot{S}})p_{\dot{R}}p_{\dot{S}} + \epsilon^{\dot{R}}p_{\dot{R}}, \quad (3.13)$$

where a possible term independent of $p^{\dot{A}}$ was absorbed into T . Equation $\frac{1}{2}E_{22}^{\dot{A}\dot{B}} = \delta^{\dot{A}}(K^{\dot{B}}) + V^{\dot{A}}(k^{\dot{B}}) - 2K_{\dot{B}}\delta^{\dot{S}}Q^{\dot{A}\dot{B}}$ may now be rewritten in the standard form: $\partial^{\dot{A}}(U^{\dot{B}}) = 0$. This gives us a determination of

$$\delta^{\dot{B}}T = TF^{\dot{B}} - \frac{1}{2}(b + 4\chi_0)p_{\dot{S}}\delta^{\dot{S}}\partial^{\dot{B}}\Theta + (b + 4\chi_0)\partial^{\dot{B}}\Theta + \frac{1}{2}N^{\dot{B}}\delta^{\dot{C}}p_{\dot{C}} + \gamma p^{\dot{B}} + \zeta^{\dot{B}}. \quad (3.14)$$

Again we apply the zero operators $\delta^{\dot{A}}\partial_{\dot{A}} - \partial_{\dot{A}}\delta^{\dot{A}} + F^{\dot{A}}\partial_{\dot{A}}$ and $\delta^{\dot{A}}\partial_{\dot{A}} - V^{\dot{A}}\partial_{\dot{A}}$ to the two equations for T . After somewhat lengthy calculations one determines three new constraints on the coefficients. The first operator insists that

$$2\gamma = N^{\dot{A}}\delta_{\dot{A}} - \epsilon^{\dot{A}}_{,\dot{A}}. \quad (3.15)$$

The second one requires

$$\zeta^{\dot{A}}_{,\dot{A}} - F^{\dot{A}}\zeta_{\dot{A}} = \epsilon^{\dot{A}}N_{\dot{A}}, \quad (3.16)$$

$$2\gamma_{,\dot{A}} + 2\gamma F_{\dot{A}} + (b + 4\chi_0)N_{\dot{A}} - F^{\dot{B}}_{,\dot{B}}\epsilon_{\dot{A}} + 2N^{\dot{B}}\delta_{(\dot{B},\dot{A})} - 2(N_{(\dot{A}}\delta_{\dot{B})})^{\dot{B}} + F^{\dot{B}}N_{\dot{B}}\delta_{\dot{A}} = 0. \quad (3.17)$$

It is clear from Eq. (3.15) that γ is now determined while Eq. (3.16) puts a solvable constraint on $\zeta^{\dot{A}}$ with many solutions. Inserting the expression for γ into Eq. (3.17), the latter becomes

$$\epsilon^{\dot{B}}_{,\dot{B}}\delta_{\dot{A}} + \epsilon^{\dot{B}}_{,\dot{B}}F_{\dot{A}} + F^{\dot{B}}_{,\dot{B}}\epsilon_{\dot{A}} + 2(N_{\dot{A}}\delta_{\dot{B}})^{\dot{B}} - 2N^{\dot{B}}\delta_{\dot{B},\dot{A}} = 4\chi_0N_{\dot{A}}, \quad (3.18)$$

whose solution we will discuss with respect to the different Petrov types. However, useful pieces of it can still be separated off. We multiply by $\delta^{\dot{A}}$ and use the constraint on $\delta^{\dot{A}}$ [Eqs. (3.10) and (3.11)]. This results in

$$[(2N^{\dot{B}}\delta_{\dot{B}} + \epsilon^{\dot{B}}_{,\dot{B}})\delta^{\dot{A}} + b\epsilon^{\dot{A}}]_{,\dot{A}} = 4\chi_0N^{\dot{A}}\delta_{\dot{A}}. \quad (3.19)$$

Second, operating with $\partial/\partial q_{\dot{A}}$ we also obtain another corollary equation

$$2F^{\dot{B}}_{,\dot{B}}\epsilon^{\dot{A}}_{,\dot{A}} + \epsilon^{\dot{A}}F^{\dot{B}}_{,\dot{B}} + F^{\dot{A}}\epsilon^{\dot{B}}_{,\dot{B}} + 2N^{\dot{A}}_{,\dot{A}}\delta^{\dot{B}} + 4N^{\dot{A}}_{,\dot{A}}\delta^{\dot{B}}_{,\dot{B}} + 2N^{\dot{A}}\delta^{\dot{B}}_{,\dot{B}} - 4\chi_0N^{\dot{A}}_{,\dot{A}} = 0. \quad (3.20)$$

These constraints are necessary and sufficient for us to rewrite Eq. (3.14) as the gradient of something, which gives us the master equation. Once again it is necessary to eliminate terms of the form $(\partial^{\dot{A}}\partial^{\dot{B}}\Theta)\partial^{\dot{C}}\partial_{\dot{B}}\Theta$ by the use of the hyperheavenly equation.

At this point, we wish to use the automorphisms of the tetrad to simplify the constraint equations as much as possible. We recall⁴ that the variables $q_{\dot{A}}$ are just labels for different members of the two-dimensional congruence of (plane) null 2-surfaces which the space possesses. Therefore, transformations to new labels $q'_{\dot{R}}$ which do not affect the form (in terms of the new variables) of the tetrad, but simplify relevant equations, are very useful. In Ref. 4 we spell these out in terms of

$$dq'_{\dot{R}} = T_{\dot{R}}^{\dot{A}}dq_{\dot{A}}, \quad p'^{\dot{R}} = T^{-1}_{\dot{A}}{}^{\dot{R}}p^{\dot{A}} + \sigma'^{\dot{R}}, \quad (3.21)$$

where $T_{\dot{R}}^{\dot{A}}$ and $\sigma'^{\dot{R}}$ are independent sets of functions of $q_{\dot{A}}$ only. In the type [III] \otimes [anything], $C^{(2)} = -F^{\dot{A}}_{,\dot{A}} \neq 0$. Under these transformations it acquires a multiplicative factor of T^{-1} (the inverse of the determinant of the matrix $T_{\dot{R}}^{\dot{A}}$). We may therefore choose T to make it any constant nonzero value. We choose, therefore $C^{(2)} = -1$. This implies $F^{\dot{A}} = \frac{1}{2}q^{\dot{A}} + \xi^{\dot{A}}$. But we also have that $F'^{\dot{R}} = T^{-1}_{\dot{A}}{}^{\dot{R}}F^{\dot{A}} - (\ln T)'^{\dot{R}}$. (3.22)

It is therefore sufficient to maintain $T=1$ and to pick $q'^{\dot{R}}$ such that $q'^{\dot{R}}dq'_{\dot{R}} - q^{\dot{A}}dq_{\dot{A}} = 2d\xi$ in order to insure that $F'^{\dot{R}} = \frac{1}{2}q'^{\dot{R}}$ only. We may therefore assume that this has already been done. But, using the transformation properties of Γ_{22} , we find that

$$N'^{\dot{R}} = T^{-1}T^{-1}_{\dot{A}}{}^{\dot{R}}N^{\dot{A}} - \frac{1}{2}F'^{\dot{S}}_{,\dot{S}}\sigma'^{\dot{R}} - \frac{1}{2}\sigma'^{\dot{S}}_{,\dot{S}}F'^{\dot{R}} + \frac{1}{2}\sigma'^{\dot{S}}_{,\dot{R}}\dot{s}_{,\dot{S}}. \quad (3.23)$$

Restricting ourselves now to transformations with $T_{\dot{R}}^{\dot{A}} = \delta^{\dot{A}}_{\dot{R}}$, and setting h as any solution of the equation $q^{\dot{A}}h_{,\dot{A}} + 4h - 2N^{\dot{A}}_{,\dot{A}} = 0$, we find that a choice of $\sigma'^{\dot{R}} = -hq'^{\dot{R}} + 2h'^{\dot{R}} + 2N'^{\dot{R}}$ guarantees that $N'^{\dot{R}} \equiv 0$. Therefore, we may always assume, initially, restricting ourselves to a left-[III] space, that $F^{\dot{A}} = \frac{1}{2}q^{\dot{A}}$, $N^{\dot{A}} = 0$. (There is even still some freedom left in the gauge corresponding to the $\sigma'^{\dot{R}}$ generated by h being some homogeneous function of order -4 .)

Still remaining in a left-[III] space, we may now look at our constraint equations. Equation (3.10) gives us $\delta^{\dot{A}} = b'^{\dot{A}}$, which implies that $\delta^{\dot{A}}_{,\dot{A}} = 0$. Equation (3.11) then becomes $q^{\dot{A}}b_{,\dot{A}} = 2b$, which determines b as a homogeneous function^{1d} of order 2, therefore still having the freedom of one arbitrary function of one variable. Using $a \equiv \epsilon^{\dot{A}}_{,\dot{A}}$, Eq. (3.20) becomes $q^{\dot{A}}a_{,\dot{A}} = -4a$, which says a must be a homogeneous function of order -4 . Picking a as an arbitrary such function, Eq. (3.18) gives us a form for $\epsilon^{\dot{A}} = a'^{\dot{A}} - \frac{1}{2}aq^{\dot{A}}$.

In the case of Petrov type $[N] \otimes$ [anything]-left-[N]- we surely have $F^{\dot{A}}_{,\dot{A}} = 0$, which implies that $F^{\dot{A}}$ is a gradient, $F^{\dot{A}} = f'^{\dot{A}}$. Equation (3.22) reduces to

$$f'^{\dot{R}} = (f - \ln T)'^{\dot{R}}$$

so that, if we choose $\ln T = f$, then $f' = 0$. We may therefore assume initially that $F^{\dot{A}} \equiv 0$, restricting ourselves to those transformations that have constant T . (This reduces the hyperheavenly equation to a much more manageable form.) Equations (3.10) and (3.11) then tell us that $-b = \rho_0$, a constant, and $\delta^{\dot{A}} = \frac{1}{2}\rho_0q^{\dot{A}} + \varphi'^{\dot{A}}$, for some φ , an arbitrary function of $q_{\dot{B}}$ only. However, Eq. (3.18) reduces to

$$n\delta^{\dot{A}} + (\rho_0 - 2\chi_0)N^{\dot{A}} + (\frac{1}{2}a + N^{\dot{B}}\delta_{\dot{B}})^{\dot{A}} = 0,$$

where $n = N^{\dot{B}}_{,\dot{B}}$. This tells us of the existence of some scalar ξ such that Eqs. (2.11b) are determined.

We also note that, for plane hyperheavens with $\alpha_0 = 0$, the transformation equations for $\delta_{\dot{A}}$ and $\epsilon_{\dot{A}}$ are easily determined to be

$$\delta_{\dot{A}} = T^{-1}_{\dot{A}}{}^{\dot{R}}\delta'_{\dot{R}}, \quad \epsilon^{\dot{A}} = T^{\dot{A}}_{\dot{S}}[\epsilon'^{\dot{S}} - 2\chi_0\sigma'^{\dot{S}} + \sigma'^{\dot{R}}\delta'_{\dot{R}}{}^{\dot{S}} + \sigma'^{\dot{S}}{}_{,\dot{R}}\delta'_{\dot{R}}{}^{\dot{S}}]. \quad (3.24)$$

These transformations can be used to eliminate $\epsilon^{\dot{A}}$ if desired. Here we maintain generality, however, since, starting with some given symmetry, this particular gauge may be difficult to insure.

Before deriving the Ernst potentials associated with these Killing vectors, it is probably useful to briefly review their connection to quadratic Killing structures, presented in detail in Ref. 12. It is well known¹³ that the structure consisting of $K_{\dot{A}\dot{B}}$, $\ell_{\dot{A}\dot{B}}$, $\ell^{\dot{A}\dot{B}}$, and $\nabla^{\dot{A}}{}_{\dot{B}\dot{C}}$ is closed under differentiation. (The components of the Riemann tensor are also needed.) However, Ref. 12 looks at all the (quadratic) objects in the direct product of this structure with itself, decomposes it into objects irreducible under $SL(2, C)$, and calculates the appropriate closure relations. Two of the most important such irreducible objects are the two 1-forms G and \bar{G} defined by

$$G = -\ell_{\dot{A}\dot{B}}K^{\dot{B}}{}_{\dot{C}}g^{\dot{C}\dot{A}}, \quad \bar{G} = -\ell^{\dot{A}\dot{B}}K_{\dot{C}}{}^{\dot{B}}g_{\dot{A}}{}^{\dot{C}}. \quad (3.25)$$

It is shown that, in vacuum with $\chi_0 = 0$, both are closed forms. We may therefore infer, in some appropriate neighborhood, the existence of some potentials \mathcal{E} , $\bar{\mathcal{E}}$ such that $d\mathcal{E} = G$, $d\bar{\mathcal{E}} = \bar{G}$. We also have the useful relation, $K^{\mu}K_{\mu} + \frac{1}{2}\mathcal{E} + \frac{1}{2}\bar{\mathcal{E}}$ equals a constant, which may always be chosen zero. The equation for $*d^*G$ then becomes the usual nonlinear equation which \mathcal{E} is required to satisfy.⁵

Using $d\mathcal{E} = e_{\dot{B}}\delta^{\dot{B}}\mathcal{E} - E^{\dot{B}}\partial_{\dot{B}}\mathcal{E}$, we obtain, for our tetrad,

$$\begin{aligned} \frac{1}{2}\partial_{\dot{B}}\mathcal{E} &= \ell_{11}K_{\dot{B}} - \ell_{12}k_{\dot{B}}, & \frac{1}{2}\delta^{\dot{B}}\mathcal{E} &= \ell_{22}k^{\dot{B}} - \ell_{12}K^{\dot{B}}, \\ \frac{1}{2}\partial_{\dot{B}}\bar{\mathcal{E}} &= -\ell_{\dot{B}\dot{A}}k^{\dot{A}}, & \frac{1}{2}\delta^{\dot{B}}\bar{\mathcal{E}} &= -\ell^{\dot{B}\dot{A}}K_{\dot{A}}. \end{aligned} \quad (3.26)$$

For left-flat spaces, we use the forms derived above and easily find that $\frac{1}{2}\mathcal{E} = 2\alpha_0 T - \rho_0 \delta_{\dot{A}} p^{\dot{A}} + \tau$, where τ is a function of $q_{\dot{B}}$ only. Inserting this into the equation for $\frac{1}{2}\delta^{\dot{B}}\mathcal{E}$ and using the known form of $\delta^{\dot{B}}T$ we easily find the form given for τ in Eq. (2.12b). Using $-\ell_{\dot{B}\dot{A}} = 2\partial_{\dot{B}}K_{\dot{A}} = 2\partial_{\dot{B}}\partial_{\dot{A}}T$ and the form for $k^{\dot{A}}$, the equations for $\bar{\mathcal{E}}$ may be determined by the same method, or from the equation $K^{\mu}K_{\mu} + \frac{1}{2}\mathcal{E} + \frac{1}{2}\bar{\mathcal{E}} = 0$. The case of other plane hyperheavens proceeds similarly. We note that $\ell_{11} = 0$, $\ell_{12} = -b$, $\ell_{22} = -b_{,\dot{A}}p^{\dot{A}} + 2N^{\dot{A}}\delta_{\dot{A}} - \epsilon^{\dot{A}}_{,\dot{A}}$, from which $\frac{1}{2}\mathcal{E} = b\delta_{\dot{B}}p^{\dot{B}} + \nu$ is trivial— ν a function of $q_{\dot{B}}$ only. Using Eqs. (3.7) and (3.8) for $K^{\dot{A}}$ and T , we may rewrite

$$K^{\dot{A}} = \delta_{\dot{B}}Q^{\dot{A}\dot{B}} - p_{\dot{B}}\delta^{\dot{B},\dot{A}} - 2\chi_0 p^{\dot{A}} - \epsilon^{\dot{A}}, \quad (3.27)$$

which, inserted into the equation for $\frac{1}{2}\delta^{\dot{B}}\bar{\mathcal{E}}$ with $\chi_0 = 0$, gives the equation for $\nu^{\dot{A}}$ in Eq. (2.12a). However, again with $\chi_0 = 0$, Eq. (3.19) assures us that this equation always has a solution. For a left-[III] space Eqs. (2.11a) inserted into Eq. (3.19) tell us that $\nu^{\dot{A}} = b(a^{\dot{A}} - \frac{1}{2}aq^{\dot{A}}) + ab_{,\dot{A}} = (ab)_{,\dot{A}} - \frac{1}{2}abq^{\dot{A}}$, from which we see that $\nu - ab$ is a homogeneous function of order 0 while, of course, ab is homogeneous of order -2. For a left-[N] space, Eq. (2.11b) for $\delta^{\dot{A}}$ and Eq. (3.19) with $\chi_0 = 0$ give us the existence of ν as well as an explicit relation with $\epsilon^{\dot{A}}$,

$$\rho_0 \epsilon^{\dot{A}} + 2\xi \delta^{\dot{A}} + \nu^{\dot{A}} = 0.$$

4. KILLING SPINORS

We are here interested in Killing spinors of type $D(0, k)$, $k = \frac{1}{2}, 1, \frac{3}{2}, \dots$. For simplicity most of the discussion will be restricted to left-flat spaces where it is easier to see the relevant structures. We note that such a Killing spinor, $L_{A\dots K}$ satisfies⁷

$$\nabla_{(R} \dot{\tau} L_{A\dots K)} = 0 \quad \text{or} \quad \nabla_R \dot{\tau} L_{A\dots K} = \epsilon_{R(A} \ell^{\dot{\tau}}{}_{B\dots K)}. \quad (4.1)$$

In pure vacuum—the Ricci tensor vanishes—the integrability conditions become

$$\nabla_{(A} (\ell^{\dot{R}}{}_{\dot{\tau}})_{B\dots K)} = 0, \quad L_{N(A\dots J} C^N{}_{KUV)} = 0 \quad (4.2)$$

so that $\ell^{\dot{\tau}}{}_{B\dots}$ is also a Killing spinor.

Using our standard tetrad in a left-flat space— $F^{\dot{A}} = 0 = N^{\dot{A}}$ —the operator $\nabla_R \dot{\tau}$ acting on objects with all undotted indices gives the same result as $\partial_R \dot{\tau} = -\sqrt{2}(\delta_R^1 \partial^{\dot{\tau}} + \delta_R^2 \delta^{\dot{\tau}})$. We label the various components of $L_{A\dots K}$ by $L_{(j)}$ where $j = 0, 1, \dots, 2k$, indicates how many of the indices have the value 2; i. e., $L_{(0)} = L_{1\dots 1}$, $L_{(1)} = L_{1\dots 12}, \dots, L_{(k)} = L_{2\dots 2}$. The determining equations (4.1) may then be written as the set of $2k+2$ equations

$$(2k+1-j)\partial^{\dot{\tau}} L_{(j)} = -j\partial^{\dot{\tau}} L_{(j-1)}, \quad j = 0, \dots, 2k+1. \quad (4.3)$$

We note that the first of these equations merely insists that $L_{(0)}$ is independent of $p^{\dot{A}}$ so that there are plenty of solutions. If we pick $L_{(0)}$ as a —some specific function of $q_{\dot{B}}$ —the next equation is then $k\partial^{\dot{\tau}} L_{(1)} = -\frac{1}{2}a^{\dot{\tau}}$, determining

$$L_{(1)} = -(a^{\dot{\tau}} p_{\dot{\tau}} + b)/2k, \quad (4.4)$$

where b is some new function of $q_{\dot{B}}$ only.

We now note that the existence of a complete solution starting with a given choice of such an a and b is guaranteed: Given a particular sequence up to and including $L_{(j)}$, for some $j \geq 1$, the condition for the existence of $L_{(j+1)}$ is seen to be $\partial^{\dot{\tau}} \delta^{\dot{\tau}} L_{(j)} = 0$. But this is just the vanishing of $\delta^{\dot{\tau}} \partial^{\dot{\tau}} L_{(j)} = -[j/(2k+j-1)]\delta^{\dot{\tau}} \delta^{\dot{\tau}} L_{(j-1)} = 0$. Therefore, the existence of $L_{(j+1)}$ is assured. Moreover, the last equation is just $\delta^{\dot{\tau}} L_{(2k)} = 0$, but the above argument tells us that $\partial^{\dot{\tau}} \delta^{\dot{\tau}} L_{(2k)} = 0$. Therefore, there exists N such that $0 = \delta^{\dot{\tau}} L_{(2k)} = \partial^{\dot{\tau}} N$, which gives us a final constraint on the manifold in the form of $N = f(q_{\dot{B}})$, where N is clearly dependent on $2k-1$ previously determined functions of $q_{\dot{B}}$ only—“constants of the integration procedure,”—and the key function Θ . It is quite interesting that, in the process of determining N , we discover a hierarchy of key functions associated with Θ , and determined by it via the heavenly equation and its various prolongations. This hierarchy was first discovered by Boyer and Plebański.³ Here we will give a brief review of the relevant notation and explain how it enters into the calculation of our Killing spinors. We start with the function Θ itself which, via Eqs. (2.6), determines the existence of Λ , a “first integral of the heavenly equation.” Thinking of Θ as a function of $p^{\dot{A}}$ and $q_{\dot{B}}$, we may, following Ref. 3, give names to the partial derivatives of Θ ¹⁴ by writing

$$d\Theta = r_{\dot{A}} dq^{\dot{A}} + s_{\dot{A}} dp^{\dot{A}}, \quad s_{\dot{A}} = \partial_{\dot{A}}\Theta, \quad r_{\dot{A}} = \Theta_{,\dot{A}}. \quad (4.5)$$

Thinking of the new quantities as new variables in an enlarged space and looking for other Pfaffians integrable when restricted to the integral variety determined

by Eq. (4.5), they found Λ such that

$$\begin{aligned} \frac{1}{2}d\Lambda &= t_{\dot{A}}dq^{\dot{A}} + r_{\dot{A}}dp^{\dot{A}} + \frac{1}{2}s_{\dot{A}}ds^{\dot{A}}, \\ \frac{1}{2}\partial_{\dot{A}}\Lambda &= r_{\dot{A}} + \frac{1}{2}s_{\dot{B}}\partial_{\dot{A}}s^{\dot{B}}, \quad \frac{1}{2}\Lambda_{,\dot{A}} = t_{\dot{A}} + \frac{1}{2}s_{\dot{B}}s^{\dot{B}}_{,\dot{A}}, \end{aligned} \quad (4.6)$$

where the $t_{\dot{A}}$ are new spinors defined by this equation. [It can be checked that this is the same Λ determined by Eq. (2.6b).] This sequence is found to continue, each time the new one being determined by the old spinors and introducing one new spinor—new variables in the prolongation space. The next two are determined by

$$\begin{aligned} d\Xi &= u_{\dot{A}}dq^{\dot{A}} + t_{\dot{A}}dp^{\dot{A}} + r_{\dot{A}}ds^{\dot{A}}, \\ d\Upsilon &= v_{\dot{A}}dq^{\dot{A}} + u_{\dot{A}}dp^{\dot{A}} + t_{\dot{A}}dp^{\dot{A}} + \frac{1}{2}r_{\dot{A}}dr^{\dot{A}}. \end{aligned} \quad (4.7)$$

By introducing some labels we can easily write the entire sequence in a compact form. We define $\Omega_{(\ell)}$, $\ell = 2, 3, \dots$, and $\Psi_{(j)}^{\dot{A}}$, $j = -\frac{1}{2}, +\frac{1}{2}, \frac{3}{2}, \dots$:

$$\begin{aligned} \Omega_{(2)} &= \Theta, & \Psi_{(-1/2)}^{\dot{A}} &= q^{\dot{A}}, & \Psi_{(7/2)}^{\dot{A}} &= t^{\dot{A}}, \\ \Omega_{(3)} &= \frac{1}{2}\Lambda, & \Psi_{(1/2)}^{\dot{A}} &= p^{\dot{A}}, & \Psi_{(9/2)}^{\dot{A}} &= u^{\dot{A}}, \\ \Omega_{(4)} &= \Xi, & & & & \\ \Omega_{(5)} &= \Upsilon, & \Psi_{(3/2)}^{\dot{A}} &= s^{\dot{A}}, & \Psi_{(11/2)}^{\dot{A}} &= v^{\dot{A}}, \\ \dots & & \Psi_{(5/2)}^{\dot{A}} &= r^{\dot{A}}, & \dots & \end{aligned} \quad (4.8)$$

Then we find that for $\ell = 2m$ or $2m + 1$, respectively,

$$\begin{aligned} d\Omega_{(2m)} &= \sum_{j=-1/2}^{m-1/2} \Psi_{(2m-j)}^{\dot{A}} d\Psi_{(j)}^{\dot{A}}, \\ d\Omega_{(2m+1)} &= \sum_{j=-1/2}^{m-1/2} \Psi_{(2m+1-j)}^{\dot{A}} d\Psi_{(j)}^{\dot{A}} + \frac{1}{2}\Psi_{(m+1/2)}^{\dot{A}} d\Psi_{(m+1/2)}^{\dot{A}}. \end{aligned} \quad (4.9)$$

Next we note the fact that is especially important to us about this hierarchy of new spinors. It is checked by straightforward but tedious calculation that the new spinors are related to the old ones in a very simple hierarchical structure,

$$\delta^{\dot{A}}\Psi_{(j)}^{\dot{B}} = \partial^{\dot{A}}\Psi_{(j+1)}^{\dot{B}}, \quad j = -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \dots \quad (4.10)$$

Then, noting that the integrations for $L_{(0)}$ and $L_{(1)}$ already performed were beginning to introduce polynomials in $p^{\dot{A}}$, we define a sequence of functions of $q_{\dot{B}}$ only,

$$\begin{aligned} a_{(i)} : a_{(0)} \equiv a, \quad a_{(1)} \equiv b, \quad \dots, \quad i = 0, 1, 2, 3, \dots, \\ a_{(-m)} \equiv 0, \quad m = 1, 2, 3, \dots \end{aligned} \quad (4.11)$$

and, thereby, some special polynomials

$$\rho_{\ell} \equiv \sum_{i=0}^{\ell} \frac{1}{(\ell-1)!} a_{(i)} \cdot \dot{A}_1 \dots \dot{A}_{\ell-i} p^{\dot{A}_1} \dots p^{\dot{A}_{\ell-1}}, \quad \ell = 0, 1, 2, \dots, \quad (4.12)$$

with $\rho_{-m} \equiv 0$, $m = 1, 2, 3, \dots$.

We may then easily derive the following useful recursion relations:

$$\begin{aligned} \partial^{\dot{A}}\rho_{\ell} &= \rho_{\ell-1}^{\dot{A}}, \\ \delta^{\dot{A}}\rho_{\ell} &= \rho_{\ell-1}^{\dot{B}}\partial^{\dot{A}}s^{\dot{B}} + \rho_{\ell}^{\dot{A}}, \\ &= \partial^{\dot{A}}[\rho_{\ell+1} + \rho_{\ell-1}^{\dot{B}}s^{\dot{B}}] - \rho_{\ell-2}^{\dot{A}}\dot{A}^{\dot{B}}s_{\dot{B}}. \end{aligned} \quad (4.13)$$

The current notation is very condensed since, for example, Eq. (4.10) with $j = \frac{1}{2}$ already includes some ten terms when rewritten in terms of Θ and Λ . However, it is just what is needed to integrate the Killing

spinor equations (4.3), using the two sets of recursion relations given in Eqs. (4.10) and (4.13). Since the method is now very straightforward, we simply give one example of a particular derivation and then general results. However, the actual form of the results is rather complicated so that we give, in addition to a general form, several specific examples. Given the equations for a $D(0, k)$ Killing spinor, the solution to Eqs. (4.3) is determined by giving all $L_{(m)}$, $m = 0, \dots, 2k$, and the final constraint equation. We find, where $\binom{k}{m}$ are the usual binomial coefficients, that

$$\begin{aligned} + L_{(0)} &= \rho_0 = a_{(0)}, \quad -\binom{2k}{1}L_{(1)} = \rho_1 = a_{(0)}, \quad k p^{\dot{A}} + a_{(1)}, \\ + \binom{2k}{2}L_{(2)} &= \rho_2 + \rho_0^{\dot{A}}s^{\dot{A}}, \\ - \binom{2k}{3}L_{(3)} &= \rho_3 + \rho_1^{\dot{A}}s^{\dot{A}} + \rho_0^{\dot{A}}r^{\dot{A}}. \end{aligned} \quad (4.14)$$

Using Eq. (4.3) with $\ell = 4$, we have

$$\begin{aligned} (2k-3)\partial^{\dot{B}}L_{(4)} &= -4\delta^{\dot{B}}L_{(3)} \\ &= 4\binom{2k}{3}^{-1} [\delta^{\dot{B}}\rho_3 + \rho_1^{\dot{A}}\delta^{\dot{B}}s^{\dot{A}} + (\delta^{\dot{B}}\rho_1^{\dot{A}})s^{\dot{A}} \\ &\quad + \rho_0^{\dot{A}}\delta^{\dot{B}}r^{\dot{A}} + (\delta^{\dot{B}}\rho_0^{\dot{A}})r^{\dot{A}}], \end{aligned}$$

or, using our recursion relations,

$$\begin{aligned} \partial^{\dot{B}}L_{(4)} &= \binom{2k}{4}^{-1} \{ \partial^{\dot{B}}[\rho_4 + \rho_2^{\dot{B}}s^{\dot{B}}] - \rho_1^{\dot{A}}\dot{A}^{\dot{B}}s_{\dot{A}} + \rho_1^{\dot{A}}\dot{A}^{\dot{B}}\partial^{\dot{B}}r^{\dot{A}} \\ &\quad + \rho_1^{\dot{A}}\dot{A}^{\dot{B}}\dot{B}^{\dot{C}}s^{\dot{A}} + \rho_0^{\dot{A}}\dot{A}^{\dot{B}}\dot{C}^{\dot{D}}\partial^{\dot{B}}s^{\dot{C}} + \rho_0^{\dot{A}}\dot{A}^{\dot{B}}\dot{C}^{\dot{D}}t^{\dot{A}} \\ &\quad + \rho_0^{\dot{A}}\dot{A}^{\dot{B}}\dot{C}^{\dot{D}}r^{\dot{A}} \} \\ &= \binom{2k}{4}^{-1} \{ \partial^{\dot{B}}[\rho_4 + \rho_2^{\dot{A}}s^{\dot{A}} + \rho_1^{\dot{A}}\dot{A}r^{\dot{A}} + \rho_0^{\dot{A}}\dot{A}t^{\dot{A}} \\ &\quad + \frac{1}{2}\rho_0^{\dot{A}}\dot{A}^{\dot{B}}\dot{C}^{\dot{D}}s^{\dot{A}}s^{\dot{C}}] - (\partial^{\dot{B}}\rho_1^{\dot{A}})r^{\dot{A}} + \rho_0^{\dot{A}}\dot{A}^{\dot{B}}r^{\dot{A}} \}, \end{aligned}$$

from which we have that

$$\begin{aligned} L_{(4)} &= \binom{2k}{4}^{-1} [\rho_4 + \rho_2^{\dot{A}}s^{\dot{A}} + \rho_1^{\dot{A}}\dot{A}r^{\dot{A}} \\ &\quad + \rho_0^{\dot{A}}\dot{A}t^{\dot{A}} + \frac{1}{2}\rho_0^{\dot{A}}\dot{A}^{\dot{B}}\dot{C}^{\dot{D}}s^{\dot{A}}s^{\dot{C}}]. \end{aligned} \quad (4.15)$$

Continuing in this way we acquire the general form

$$\begin{aligned} M_{(\ell)} &\equiv (-1)^{\ell} \binom{2k}{\ell} L_{(\ell)} \\ &= \rho_{\ell} + \sum_{n=1}^{[\ell/2]} \frac{1}{n!} \sum_{m_1, \dots, m_n=0}^{\ell-2n} \rho_{\ell-M-2n, \dot{A}_1 \dots \dot{A}_n} \\ &\quad \times \Psi_{(\dot{A}_1/2+m_1)}^{\dot{A}_1} \dots \Psi_{(\dot{A}_n/2+m_n)}^{\dot{A}_n}, \end{aligned} \quad (4.16)$$

where $[\ell/2]$ means the greatest integer in $\ell/2$ and $M \equiv \sum_{i=1}^n m_i$. This is the form which is given naturally by the method of solving the equations with $q_{\dot{A}}$ and $p^{\dot{B}}$ as the independent variables. However, the $p^{\dot{B}}$ are just $\Psi_{(1/2)}^{\dot{B}}$. Therefore, we can rewrite Eq. (4.16) in the simpler form,

$$\begin{aligned} (-1)^{\ell} \binom{2k}{\ell} L_{(\ell)} &= a_{(\ell)} + \sum_{n=1}^{\ell} \frac{1}{n!} \\ &\quad \times \sum_{m_1, \dots, m_n=0}^{\ell-n} \left(a_{(\ell-M-n)} \Psi_{(\dot{A}_1/2+m_1)}^{\dot{A}_1} \dots \Psi_{(\dot{A}_n/2+m_n)}^{\dot{A}_n} \right). \end{aligned} \quad (4.17)$$

Next, we recall that the last of Eqs. (4.3) says that $\delta^{\dot{A}} L_{(2k)} = 0$. In the formulation given above, this constraint can be rewritten to simply say that $0 = N - f(q_{\dot{B}}) = M_{(2k+1)}$. This, then, becomes the master constraint equation—connecting the components $a_{(i)}$ and the functions of Θ —which determines the existence of any particular Killing spinor in our left-flat space, and is the analog of our master equation for Killing vectors. In particular, note that the existence of a $D(0, 1)$ Killing spinor implies (in vacuum) a $D(\frac{1}{2}, \frac{1}{2})$ Killing spinor by Eqs. (4.2). Therefore, the conditions for existence of a $D(0, 1)$ Killing spinor should be equivalent or a subset of the condition for existence of a Killing vector—a $D(\frac{1}{2}, \frac{1}{2})$ Killing spinor. But the $D(0, 1)$ condition, for L_{AB} , would be that $M_{(3)} = 0$. Comparing the form of $L_{(3)}$ given by Eq. (4.14) with the master Killing vector equation, Eqs. (2.8) and (2.9), we see that it is indeed a subcase of Eq. (2.9) corresponding to $\alpha_0 = 0 = \rho_0 = \chi_0 = \gamma_0$.

The simplest case is just that of a $D(0, \frac{1}{2})$ Killing spinor in which the master equation is just

$$M_{(2)} = 0 \quad \text{or} \quad a_{0, \dot{A}} \partial^{\dot{A}} \Theta = \frac{1}{2} a_{0, \dot{A}\dot{B}} \dot{p}^{\dot{A}} \dot{p}^{\dot{B}} + a_{1, \dot{A}} \dot{p}^{\dot{A}} + a_2 = \rho_2. \quad (4.18)$$

We quickly see that this implies that $0 = a_{0, \dot{A}} \partial^{\dot{A}} \dot{p}^{\dot{B}} \dot{p}^{\dot{C}} \dot{p}^{\dot{D}} \Theta = a_{0, \dot{A}} \dot{C}^{\dot{A}\dot{B}\dot{C}\dot{D}}$. For a_0 nonconstant, this implies that $a_{0, \dot{A}}$ determines a quadruply degenerate Debever–Penrose vector and insures that the space is of type $[\text{III}, N \text{ or } -] \otimes [\bar{N}]$.

We also note that a constant $D(0, k)$ Killing spinor always exists in a left-flat space, for any k . It is of the form $L_{(j)} = a_{(j)}$, where all of the $a_{(j)}$ are constant. (The constraint equation is automatically satisfied.)

5. CONCLUSIONS

The results presented here show a rather amazing feature of the symmetries of plane hyperheavens. Their description is simpler than the corresponding description of pure heavens since the troublesome constant α_0 (from heavens) vanishes in hyperheavens, thereby eliminating the necessity of introducing the higher key function Λ . The simple, succinct form of the master equation in plane hyperheavens makes it clear that an explicit derivation of the function Θ corresponding to a spacetime with any particular set of desired symmetries should not be particularly difficult. It is therefore clear that the results of this paper, among other things, can be considered as the key to the study of all those generalized Robinson–Trautman solutions which are plane from both sides—therefore, nontwisting and nonexpanding—but with these two sides not necessarily being complex conjugates of each other.

Also we have found explicit forms for master equations determining the existence of $D(0, k)$ Killing spinors in left-flat spaces, as well as explicit forms for all the components. These equations needed the introduction of a hierarchy of key functions—a sequence of “higher integrals” of the heavenly equation—and an associated hierarchy of spinors which allow us to represent con-

cisely the components of our Killing spinors. The geometrical meaning of an arbitrary Killing spinor is still unclear, as is the full meaning of the process of prolongation of the differential structure of a spacetime. We have surely shown, however, that the two are closely connected, which we hope will assist in the better understanding of both.

We have not attempted here to discuss applications of this formalism to any particular case. For pure heavens several interesting examples were already given in Ref. 2. Similar procedures can easily be done for these plane hyperheavens; however, these will be published later in a separate study.

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³C. P. Boyer and J. F. Plebański, J. Math. Phys. 18, 1022 (1977).

⁴J. D. Finley, III and J. F. Plebański, J. Math. Phys. 17, 2207 (1976).

⁵F. J. Ernst, J. Math. Phys. 15, 1409, 2027 (1974).

⁶W. Kinnersley, J. Math. Phys. 14, 651 (1973).

⁷For a basic discussion of Killing spinors in a similar notation see S. Hacyan and J. F. Plebański, J. Math. Phys. 16, 2203 (1976). Also see the earlier discussions given in M. Walker and R. Penrose, Commun. Math. Phys. 18, 265 (1970) and L. P. Hughston, R. Penrose, P. Sommers, and M. Walker, Commun. Math. Phys. 27, 303 (1972).

⁸We use the null tetrad convention of G. C. Debney, R. P. Kerr, and A. Schild, J. Math. Phys. 10, 1842 (1969): $e^1 \cdot e^2 = +1 = e^3 \cdot e^4$, with all the other scalar products vanishing. The spinor mapping is

$$g^{A\dot{B}} = (2)^{1/2} \begin{bmatrix} e^4 & e^2 \\ e^1 & -e^3 \end{bmatrix},$$

as for example, in J. F. Plebański, J. Math. Phys. 16, 2395 (1975).

⁹We do not use the Θ gauged as in the main body of Ref. 4, but rather the one given in Appendix B, there. This is also the same gauge as used in J. D. Finley, III and J. F. Plebański, J. Math. Phys. 18, 1662 (1977).

¹⁰With $q_1^* = v$, $q_2^* = u$, one may write an arbitrary homogeneous function of degree n in the form $[uf(v/u)]^n$, where f is any sufficiently smooth function of one variable. A more covariant approach would be to pick any pair of constant basis spinors, $\lambda^{\dot{A}}$, $\zeta^{\dot{B}}$ such that $\lambda^{\dot{A}} \zeta_{\dot{A}} = 1$. Then our homogeneous function takes the form $[\lambda^{\dot{A}} q_{\dot{A}} g(\zeta^{\dot{B}} q_{\dot{B}} / \lambda^{\dot{C}} q_{\dot{C}})]^n$, where, again, g is any function of one variable.

¹¹It is worth comparing these few lines with the derivation given in Ref. 2. At that time we were unaware of this clearly superior notation and approach.

¹²F. J. Ernst and J. F. Plebański, “Killing Structures and Complex E -Potentials” Ann. Phys. (N.Y.) 107, 266 (1977).

¹³L. P. Eisenhart, *Riemannian Geometry* (Princeton U.P., Princeton, N.J., 1966), p. 238.

¹⁴The notation used here is very slightly different from that of Ref. 3, with regard to factors and signs. Reference 3 used Λ to refer to what would be $\frac{1}{2}\Lambda$ in Ref. 4. In addition there are several missing minus signs in Ref. 3, which have been corrected here.

The quantum mechanical Poincaré and Galilei groups^{a)}

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Second countable locally compact representation groups for the Poincaré group (resp. for the Galilei group) and for some of its subgroups are constructed in the "quantum mechanical case," i.e., when time and space-time inversions are assumed to be represented by antiunitary operators. The question of their uniqueness up to topological group isomorphisms is investigated.

I. INTRODUCTION

The role of $ISL(2, C)$ [the inhomogeneous $SL(2, C)$] in relativistic quantum mechanics is hardly overestimated: Its continuous unitary representations (CU-reps) on separable complex Hilbert spaces are needed in order to describe the relativistic space-time transformations of quantum mechanical states. However, it should not be forgotten that the relevant space-time symmetry group in this context is P_0 , the neutral component of the Poincaré group P , and not $ISL(2, C)$ which occurs only as a representation group¹ (hence, essentially, as a mathematical device) in the theory of continuous unitary projective representations (CUP-reps) of P_0 . In other words, the CUP-reps of P_0 are "linearized" by CU-reps of $ISL(2, C)$.

In the present paper, we also consider space and time inversions and apply the results of Ref. 1 to determine representation groups for P and for its subgroups P' (the orthochronous Poincaré group), P_+ (the proper Poincaré group), $P_{\pm}^{\pm} = P' \cup P_{\pm}'$ (the orthochronous Poincaré group) in the "quantum mechanical case," namely, when time and space-time inversions are assumed to be represented by antiunitary operators.² If G is any one of the groups P_0 , P' , P_+ , P_{\pm}^{\pm} , P (that we call globally the *Poincaré groups*), a "quantum mechanical" representation group for G will be called a *quantum mechanical G-group*. Our "quantum mechanical P-group" is not the "quantum mechanical Poincaré group" considered sometimes in the literature.³ Its meaning for G is the same as that of $ISL(2, C)$ for P_0 . In particular, all "quantum mechanical" CUA-reps of P can be obtained from (ordinary) CUA-reps of one quantum mechanical P-group (Ref. 1, Proposition 1) instead of using eight^{4,5} or four^{6,7} nonisomorphic groups as it is customary. We also consider the *Galilei groups* G_0 , G' , G_+ , G_{\pm}^{\pm} , G , i.e., the nonrelativistic space-time transformation groups corresponding to the Poincaré groups, and study their "quantum mechanical" second countable locally compact representation groups (again called the *quantum mechanical G-groups*, where G now runs through the Galilei groups). We show that, if G belongs to the Poincaré or Galilei groups and is different from P' , P , G' , and G , it admits a unique quantum mechanical G-group up to topological group isomorphisms.

The paper is organized as follows. In Sec. II, the relevant cohomology groups are determined and corresponding selectors are chosen. The quantum mechanical groups are constructed in Sec. III and the question of their uniqueness is investigated. For the sake of completeness, we also treat the known cases of P_0 ^{8,9} and G_0 .¹⁰ Two results of more general character needed in the present paper, one concerning cohomology groups of degree 2 of semidirect products of groups and the other the uniqueness of representation groups, are given in the appendices.

Results, conventions, terminology, and the notation of Ref. 1 are used throughout the paper.

II. THE COHOMOLOGY GROUPS

Our goal is now to determine the cohomology groups $H_B^2(G, U(1)_{\Phi_N})$, where G runs through the Poincaré groups and the Galilei groups and N is the biggest subgroup of G which does not include time and space-time inversions. Meanwhile, for each G , we choose a $(G, N)_B$ -selector s and a second countable locally compact group topology on $H_B^2(G, U(1)_{\Phi_N})$ such that $ev_{(g, g')}$ is continuous for all g, g' in G when $s(H_B^2)$ is equipped with the topology transported via s and $s(H_B^2)^{\wedge}$ with the corresponding compact open one.

A. The Poincaré groups

The elements of P are of the form (t, Λ) , where t is a space-time translation and Λ belongs to the Lorentz group L . As usual, Greek (resp. Latin) indices are space-time (resp. space) indices and we follow the summation convention on repeated indices. We denote by V the subgroup $\{e, \bar{e}, e', \bar{e}'\}$ of L (isomorphic to the Klein 4-group), where $e = e_L$, \bar{e} is the space inversion, e' is the time inversion, and \bar{e}' is the space-time inversion. Then P (resp. P' , resp. P_+ , resp. P_{\pm}^{\pm}) is a topological semidirect product of V (resp. of $\bar{V} = \{e, \bar{e}\}$, resp. of $\bar{V}' = \{e, \bar{e}'\}$, resp. of $V' = \{e, e'\}$) by P_0 and N is the subgroup P' (resp. P' , resp. P_0 , resp. P_0) of P .

(A. 1) P_0 : It is well known⁸ that

$$H_B^2(P_0, U(1)_I) \approx C_2,$$

where C_2 is any cyclic group of order 2, so that we can identify the group $H_B^2(P_0, U(1)_I)$ with the (multiplicative) group $\{1, -1\}$.

Now let ρ_{L_0} be the covering projection of $SL(2, C)$ onto the neutral component L_0 of L , and let σ be the normalized locally continuous Borel section associated with ρ_{L_0} defined by taking limits of

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$\sigma(\Lambda) = (1/M)(\Lambda^3_s \tau_0 + (\Lambda^j_0 + \Lambda^0_j - i\epsilon_{jkl} \Lambda^k_l) \tau_j)$, ($\Lambda^3_s \neq 0$), where

$$M^2 = 4 - \text{Tr}(\Lambda^2) + (\text{Tr}\Lambda)^2 - i\epsilon^{3kl} \Lambda^k_l \Lambda^l_k$$

and the square root $M^2 \rightarrow M$ in \mathbb{C} is chosen to be Borel in \mathbb{C} and the principal branch in the complement of the negative real half-line [cf. Ref. 4, (1.8)]. Here, τ_0 is the unit 2×2 matrix and τ_j ($1 \leq j \leq 3$) are the Pauli matrices. There is then a nontrivial element μ_0 of $Z^2_B(\mathbb{P}_0, \mathbf{U}(1)_I)$ with values in $\{1, -1\}$ such that

$$\mu_0((t, \Lambda), (t', \Lambda')) \tau_0 = \sigma(\Lambda) \sigma(\Lambda') \sigma(\Lambda \Lambda')^{-1} \quad (\text{II. 1})$$

for all $(t, \Lambda), (t', \Lambda')$ in \mathbb{P}_0 , and we define the $(\mathbb{P}_0)_B$ -selector s by $s(-1) = \mu_0$. The chosen topology on $H^2_B(\mathbb{P}_0, \mathbf{U}(1)_I)$ is obviously the discrete one. We identify the groups $s(H^2_B)^{\wedge}$ and $\{1, -1\}$, so that then $\text{ev}^s = \mu_0$, where μ_0 is considered here as a mapping of $\mathbb{P}_0 \times \mathbb{P}_0$ into $\{1, -1\}$. This convention will be tacitly followed hereafter for all cocycles with values in $\{1, -1\}$.

(A. 2) \mathbb{P}' : If $\Lambda \in \mathbb{L}_0$ and $\bar{\Lambda} = \bar{e} \Lambda \bar{e}$, then $\bar{\Lambda}^0_0 = \Lambda^0_0$, $\bar{\Lambda}^0_j = -\Lambda^0_j$, $\bar{\Lambda}^j_0 = -\Lambda^j_0$, and $\bar{\Lambda}^k_l = \Lambda^k_l$ for $1 \leq j, k, l \leq 3$. It follows that $\sigma(e \Lambda e) = \sigma(\Lambda)^{*^{-1}}$ and therefore we have

$$\hat{\Gamma}^2_Z(\bar{e}) \mu_0 = \mu_0, \quad (\text{II. 2})$$

where μ_0 is as in (A. 1) and the notation of Ref. 11, Sec. 4 has been used. Furthermore, $H^2(\bar{V}, \mathbf{U}(1)_I)$ is trivial because

$$Z^2(\bar{V}, \mathbf{U}(1)_I) = B^2(\bar{V}, \mathbf{U}(1)_I) \approx \mathbf{U}(1).$$

Since $Z^1_c(\mathbb{P}_0, \mathbf{U}(1)_I)$ is trivial and so, by Proposition A (see Appendix A),

$$H^2_B(\mathbb{P}', \mathbf{U}(1)_I) \approx H^2_B(\mathbb{P}_0, \mathbf{U}(1)_I)^{\bar{V}} \times H^2(\bar{V}, \mathbf{U}(1)_I),$$

we again have

$$H^2_B(\mathbb{P}', \mathbf{U}(1)_I) \approx C_2$$

by reason of (II. 2). As in (A. 1), we identify $H^2_B(\mathbb{P}', \mathbf{U}(1)_I)$ and $s(H^2_B)^{\wedge}$ with $\{1, -1\}$, we put the discrete topology on these groups, and we define the $(\mathbb{P}')_B$ -selector s by $s(-1) = \mu$, where (Ref. 11, Lemma 2)

$$\bar{\mu}((t, \Lambda v), (t', \Lambda' v')) = \mu_0((t, \Lambda), (t', v \Lambda' v'))$$

for all $(t, \Lambda), (t', \Lambda')$ in \mathbb{P}_0 and all v, v' in \bar{V} , with μ_0 given by (II. 1). Then $\text{ev}^s = \mu$.

(A. 3) \mathbb{P}_+ : As $\bar{e}' \Lambda \bar{e}' = \Lambda$ for all $\Lambda \in \mathbb{L}_0$, we have $(\hat{\Phi}_{\mathbb{P}_0})^2(\bar{e}') \mu_0 = \mu_0$ when μ_0 is given by (II. 1). Moreover, $H^2(\bar{V}', \mathbf{U}(1)_{\Phi_{\mathbb{P}_0}}) \approx C_2$ because $Z^2(\bar{V}', \mathbf{U}(1)_{\Phi_{\mathbb{P}_0}}) \approx C_2$ and the unique 2-coboundary is the trivial one. Proceeding as in (A. 2), we see that

$$H^2_B(\mathbb{P}_+, \mathbf{U}(1)_{\Phi_{\mathbb{P}_0}}) \approx C_2 \times C_2,$$

we identify it with $\{1, -1\}^2$ and equip it with the discrete topology. The $(\mathbb{P}_+, \mathbb{P}_0)_B$ -selector s is defined by choosing $s(-1, 1) = \bar{\mu}'_1$ and $s(1, -1) = \bar{\mu}'_2$, where

$$\bar{\mu}'_1((t, \Lambda v), (t', \Lambda' v')) = \mu_0((t, \Lambda), (t', \Lambda')),$$

$$\bar{\mu}'_2((t, \Lambda v), (t', \Lambda' v')) = \begin{cases} -1 & \text{if } v = v' = \bar{e}', \\ 1 & \text{otherwise} \end{cases}$$

for all $(t, \Lambda), (t', \Lambda')$ in \mathbb{P}_0 and all v, v' in \bar{V}' , with μ_0 given by (II. 1). We identify the groups $s(H^2_B)^{\wedge}$ and $\{1, -1\}^2$ so that, if the mapping

$$\bar{\mu}' : \mathbb{P}_+ \times \mathbb{P}_+ \rightarrow \{1, -1\}^2$$

is defined by $\bar{\mu}' = (\bar{\mu}'_1, \bar{\mu}'_2)$, then $\text{ev}^s = \bar{\mu}'$.

(A. 4) \mathbb{P}'_{\pm} : Since, for each $\Lambda \in \mathbb{L}_0$, $e' \Lambda e' = \bar{e} \Lambda \bar{e}$, and as $H^2(V', \mathbf{U}(1)_{\Phi_{\mathbb{P}'}}) \approx C_2$, we have

$$H^2_B(\mathbb{P}'_{\pm}, \mathbf{U}(1)_{\Phi_{\mathbb{P}'}}) \approx C_2 \times C_2.$$

Now we can adopt the result of (A. 3), writing μ'_i (resp. μ') instead of $\bar{\mu}'_i$ (resp. of $\bar{\mu}'$) ($i=1, 2$), taking v, v' in V' , and changing the definition of $\bar{\mu}'_1$ to

$$\mu'_1((t, \Lambda v), (t', \Lambda' v')) = \mu_0((t, \Lambda), (t', v \Lambda' v)).$$

(A. 5) \mathbb{P} : Taking account of the previous results, we have by Proposition A

$$H^2_B(\mathbb{P}, \mathbf{U}(1)_{\Phi_{\mathbb{P}}}) \approx C_2 \times C_2 \times C_2$$

because $H^2(V, \mathbf{U}(1)_{\Phi_{\mathbb{P}}}) \approx C_2 \times C_2$ [cf., for example, (Ref. 6, Lemma 5.3)]. We identify the groups $H^2_B(\mathbb{P}, \mathbf{U}(1)_{\Phi_{\mathbb{P}}})$, $s(H^2_B)^{\wedge}$, and $\{1, -1\}^3$, equip them with the discrete topology, and define the $(\mathbb{P}, \mathbb{P}')_B$ -selector s by choosing $s(-1, 1, 1) = \mu_1$, $s(1, -1, 1) = \mu_2$, $s(1, 1, -1) = \mu_3$, where

$$\mu_1((t, \Lambda v), (t', \Lambda' v'))$$

$$= \mu_0((t, \Lambda), (t', v \Lambda' v)),$$

$$\mu_2((t, \Lambda v), (t', \Lambda' v'))$$

$$= \begin{cases} -1 & \text{if } (v, v') \in \{(e', \bar{e}), (e', e'), (\bar{e}', \bar{e}), (\bar{e}', e')\}, \\ 1 & \text{otherwise,} \end{cases}$$

$$\mu_3((t, \Lambda v), (t', \Lambda' v'))$$

$$= \begin{cases} -1 & \text{if } (v, v') \in \{(e', \bar{e}), (e', \bar{e}'), (\bar{e}', \bar{e}), (\bar{e}', \bar{e}')\}, \\ 1 & \text{otherwise} \end{cases}$$

for all $(t, \Lambda), (t', \Lambda')$ in \mathbb{P}_0 and all v, v' in V , with μ_0 given by (II. 1) [cf. Ref. 6, Lemma 5.3, Table (ii)]. It follows that $\text{ev}^s = \mu$, where the 2-cocycle

$$\mu : \mathbb{P} \times \mathbb{P} \rightarrow \{1, -1\}^3$$

is defined by $\mu = (\mu_1, \mu_2, \mu_3)$.

B. The Galilei groups

We identify as usual every element g of the Galilei group \mathbf{G} with a 5-tuple $(\epsilon_g, t_g^0, \mathbf{t}_g, \mathbf{v}_g, O_g)$, where $\epsilon_g \in \{1, -1\}$, $t_g^0 \in \mathbb{R}$, $\mathbf{t}_g \in \mathbb{R}^3$, $\mathbf{v}_g \in \mathbb{R}^3$, $O_g \in \mathbf{O}(3, \mathbb{R})$ are, respectively, the time inversion, time translation, space translation, Galilean boost, and orthogonal transformation parameters. If the subgroups V, \bar{V}, \bar{V}' , and V' of \mathbf{G} are defined as in the case of the Poincaré group, we have that the Galilei groups are topological semidirect products of these subgroups by \mathbf{G}_0 exactly as in Sec. IIA with the symbol "G" instead of "P."

(B. 1) \mathbf{G}_0 : A well-known result of Bargmann (Ref. 9, 6f, 6g) tells us that

$$H^2_B(\mathbf{G}_0, \mathbf{U}(1)_I) \approx \mathbb{R} \times C_2$$

and that, for each $r \in \mathbb{R}$, we have an element μ'_0 of $Z^2_B(\mathbf{G}_0, \mathbf{U}(1)_I)$ given by $\mu'_0(g, g') = \exp(-ir\eta_0(g, g'))$, where [Ref. 9, (6.30a)]

$$\eta_0(g, g') = \mathbf{t}_g \cdot O_g \mathbf{v}_{g'} - t_g^0 (\frac{1}{2} \mathbf{v}_{g'}^2 + \mathbf{v}_g \cdot O_g \mathbf{v}_{g'}),$$

the dot denoting the scalar product on \mathbb{R}^3 . If the real numbers r and r' are different, then $[\mu'_0] \neq [\mu'_0]$. There also exists an element μ_0 of $Z^2_B(\mathbf{G}_0, \mathbf{U}(1)_I)$ with values in $\{1, -1\}$ defined by

$$\mu_0(g, g')\tau_0 = \sigma(O_g)\sigma(O_{g'})\sigma(O_g O_{g'})^{-1},$$

where σ is as in (A. 1) after an obvious identification, and one easily checks that $[\mu_0] \neq [\mu_0^r]$ for all $r \in \mathbf{R}$. We identify $H_B^2(\mathbf{G}_0, \mathbf{U}(1)_I)$ with $\mathbf{R} \times \{1, -1\}$ by means of the given group isomorphism and endow $H_B^2(\mathbf{G}_0, \mathbf{U}(1)_I)$ with the product of the canonical topology of \mathbf{R} and the discrete one on $\{1, -1\}$. The $(\mathbf{G}_0)_B$ -selector s such that $s(r, 1) = \mu_0^r$ ($r \in \mathbf{R}$) and $s(0, -1) = \mu_0$ makes $ev_{(g, g')}$ continuous for all g, g' in \mathbf{G}_0 [provided the topologies on $s(H_B^2)$ and $s(H_B^2)^{\wedge}$ are defined as stated above]. The topological groups $s(H_B^2)^{\wedge}$ and $\mathbf{R} \times \{1, -1\}$ are then identified in an obvious way, so that we have $ev^s = (\eta_0, \mu_0)$.

(B. 2) \mathbf{G}' : For each $g \in \mathbf{G}_0$, we have

$$\bar{e}(1, t_g^0, \mathbf{t}_g, \mathbf{v}_g, O_g)\bar{e} = (1, t_g^0, -\mathbf{t}_g, -\mathbf{v}_g, O_g),$$

so that $\hat{I}_Z^2(\bar{e})\mu_0^r\mu_0 = \mu_0^r\mu_0$ for all $r \in \mathbf{R}$, where μ_0^r, μ_0 are as in (B. 1). Since $Z_{\mathbf{G}_0}^1(\mathbf{G}_0, \mathbf{U}(1)_I) \approx \mathbf{R}$, it follows from Proposition A that [cf. (A. 2)]

$$H_B^2(\mathbf{G}', \mathbf{U}(1)_I) \approx \mathbf{R} \times C_2.$$

With the identification and the topology as in (B. 1), we choose the $(\mathbf{G}')_B$ -selector s such that $s(r, 1) = \bar{\mu}^r$ ($r \in \mathbf{R}$), $s(0, -1) = \bar{\mu}$, where

$$\bar{\mu}^r(gv, g'v') = \mu_0^r(g, vg'v),$$

$$\bar{\mu}(gv, g'v') = \mu_0(g, g')$$

for all g, g' in \mathbf{G}_0 and all v, v' in \bar{V} . Now we identify the topological groups $s(H_B^2)^{\wedge}$ and $\mathbf{R} \times \{1, -1\}$ and obtain $ev^s = (\bar{\eta}, \bar{\mu})$. The meaning of $\bar{\eta}$ (and of $\bar{\eta}', \eta', \eta$ in the following) should be clear.

(B. 3) \mathbf{G}_* : Since

$$\bar{e}'(1, t_g^0, \mathbf{t}_g, \mathbf{v}_g, O_g)\bar{e}' = (1, -t_g^0, -\mathbf{t}_g, \mathbf{v}_g, O_g)$$

for all $g \in \mathbf{G}_0$, we have, for each $r \in \mathbf{R}$,

$$(\hat{\Phi}_{\mathbf{G}_0})_Z^2(\bar{e}')\mu_0^r\mu_0 = \mu_0^r\mu_0. \quad (\text{II. 3})$$

Therefore,

$$H_B^2(\mathbf{G}_*, \mathbf{U}(1)_{\mathbf{G}_0}) \approx \mathbf{R} \times C_2 \times C_2,$$

and we identify it with $\mathbf{R} \times \{1, -1\}^2$ endowing it then with the product of the canonical topology of \mathbf{R} and the discrete one on $\{1, -1\}^2$. The $(\mathbf{G}_*, \mathbf{G}_0)_B$ -selector s is defined by $s(r, 1, 1) = \bar{\mu}^{r'}$ ($r \in \mathbf{R}$), $s(0, -1, 1) = \bar{\mu}_1'$, $s(0, 1, -1) = \bar{\mu}_2'$, where $\bar{\mu}^{r'}$ is defined as $\bar{\mu}^r$ but with v, v' in \bar{V}' and $\bar{\mu}_i'$ ($i=1, 2$) as in (A. 3) with g, g' in \mathbf{G}_0 instead of (t, Λ) , (t', Λ') in \mathbf{P}_0 . The topological groups $s(H_B^2)^{\wedge}$ and $\mathbf{R} \times \{1, -1\}^2$ are identified, and so we have $ev^s = (\bar{\eta}', \bar{\mu}')$, with $\bar{\mu}' = (\bar{\mu}_1', \bar{\mu}_2')$.

(B. 4) \mathbf{G}_{**} : Here we have

$$e'(1, t_g^0, \mathbf{t}_g, \mathbf{v}_g, O_g)e' = (1, -t_g^0, \mathbf{t}_g, -\mathbf{v}_g, O_g)$$

for all $g \in \mathbf{G}_0$, hence (II. 3) is also satisfied with e' instead of \bar{e}' . It follows that

$$H_B^2(\mathbf{G}_{**}, \mathbf{U}(1)_{\mathbf{G}_0}) \approx \mathbf{R} \times C_2 \times C_2,$$

and we can proceed as in (A. 4) with (B. 3) instead of (A. 3) and g, g' in \mathbf{G}_0 instead of (t, Λ) , (t', Λ') in \mathbf{P}_0 . Notice that the definition of μ_1' is the same as that of $\bar{\mu}_1'$.

(B. 5) \mathbf{G} : In analogy with (A. 5), we have

$$H_B^2(\mathbf{G}, \mathbf{U}(1)_{\mathbf{G}_0}) \approx \mathbf{R} \times C_2 \times C_2 \times C_2.$$

We identify $H_B^2(\mathbf{G}, \mathbf{U}(1)_{\mathbf{G}_0})$ with $\mathbf{R} \times \{1, -1\}^3$, equip it with the product of the canonical topology of \mathbf{R} and the discrete one on $\{1, -1\}^3$, and define the $(\mathbf{G}, \mathbf{G}')_B$ -selector s by choosing $s(r, 1, 1, 1) = \mu^r$ ($r \in \mathbf{R}$), $s(0, -1, 1, 1) = \mu_1$, $s(0, 1, -1, 1) = \mu_2$, $s(0, 1, 1, -1) = \mu_3$, where μ^r is as $\bar{\mu}^r$ but with v, v' in V ,

$$\mu_1(gv, g'v') = \mu_0(g, g')$$

for all g, g' in \mathbf{G}_0 and all v, v' in V , and μ_2, μ_3 are as in (A. 5) with g, g' in \mathbf{G}_0 instead of (t, Λ) , (t', Λ') in \mathbf{P}_0 . Then the topological groups $s(H_B^2)^{\wedge}$ and $\mathbf{R} \times \{1, -1\}^3$ are identified, and we have $ev^s = (\eta, \mu)$, with $\mu = (\mu_1, \mu_2, \mu_3)$.

III. THE REPRESENTATION GROUPS

In this section, we shall study the representation groups $s(H_B^2)_{\mathbf{G}_N} ev^s G$ for (G, N) , with the s -topology, where G, N , and s are as in the previous section. We shall follow the order of Sec. II, using the same notation. Notice that $H_B^2(G, \mathbf{R}_{\mathbf{G}_N})$ is trivial if $G \in \{\mathbf{P}_0, \mathbf{P}', \mathbf{P}_*, \mathbf{P}_{**}, \mathbf{P}\}$ and isomorphic to (the additive group of) \mathbf{R} if $G \in \{\mathbf{G}_0, \mathbf{G}', \mathbf{G}_*, \mathbf{G}_{**}, \mathbf{G}\}$ because $H^2(F, \mathbf{R}_{\mathbf{G}_N})$ is trivial for every finite group F (Ref. 12, Chap. IV, Corollary 5. 4).

A. The Poincaré groups

We recall that

$$\mathbf{ISL}(2, \mathbf{C}) = \mathbf{R}^4 \times_{\mathbf{G}} \mathbf{SL}(2, \mathbf{C}),$$

where the topological operation Φ of $\mathbf{SL}(2, \mathbf{C})$ on \mathbf{R}^4 is defined by

$$\Phi(A)x = \Gamma^{-1}(A\Gamma(x)A^*) \quad (x \in \mathbf{R}^4)$$

via the group isomorphism

$$\Gamma : x = (x^0, x^1, x^2, x^3) \mapsto \sum_{\kappa=0}^3 x^\kappa \tau_\kappa$$

of \mathbf{R}^4 onto the (additive) group of all 2×2 Hermitian matrices. The operation φ of V on $\mathbf{ISL}(2, \mathbf{C})$ such that, for each $(t, A) \in \mathbf{ISL}(2, \mathbf{C})$,

$$\varphi(\bar{e})(t, A) = (t_g, A^{*-1}),$$

$$\varphi(e')(t, A) = (t_{g'}, A^{*-1}),$$

where $t = (t^0, \mathbf{t})$, $t_g = (t^0, -\mathbf{t})$, and $t_{g'} = (-t^0, \mathbf{t})$, is topological and we have the topological semidirect product $\mathbf{ISL}(2, \mathbf{C}) \times_{\mathbf{G}} V$. We shall put $\varphi|_{\bar{V}} = \bar{\varphi}$, $\varphi|_{V'} = \varphi'$, $\varphi|_{\bar{V}'} = \bar{\varphi}'$ and tacitly consider the semidirect products relative to these operations as topological.

(A. 1) \mathbf{P}_0 : The representation group

$$\bar{\mathbf{P}}_0 = \{1, -1\}_I \mu_0 \mathbf{P}_0$$

for \mathbf{P}_0 is unique up to topological group isomorphisms by Proposition B (see Appendix B): it is THE quantum mechanical \mathbf{P}_0 -group. As mentioned in the Introduction, $\mathbf{ISL}(2, \mathbf{C})$ is a representation group for \mathbf{P}_0 : Indeed the mapping

$$(\xi, (t, \Lambda)) \mapsto (t, \xi\sigma(\Lambda)) \quad (\xi \in \{1, -1\}; (t, \Lambda) \in \mathbf{P}_0)$$

is a topological group isomorphism of $\bar{\mathbf{P}}_0$ onto $\mathbf{ISL}(2, \mathbf{C})$.

(A. 2) \mathbf{P}' : We have a representation group

$$\mathbf{P}'^{(1)} = \{1, -1\}_I \bar{\mu} \mathbf{P}'$$

for \mathbf{P}' , i. e., a quantum mechanical \mathbf{P}' -group, and a topological group isomorphism

$$(\xi, (t, \Lambda v)) \mapsto ((t, \xi\sigma(\Lambda)), v) \quad (\xi \in \{1, -1\}; (t, \Lambda) \in \mathbf{P}_0; v \in \bar{V})$$

of $\bar{\mathbf{P}}'^{(1)}$ onto $\mathbf{ISL}(2, \mathbf{C}) \times_{\bar{v}} \bar{V}$. But $\bar{\mathbf{P}}'^{(1)}$ is not the unique representation group for \mathbf{P}' up to topological group isomorphisms. To show this, we notice that by Ref. 11 (Proposition 1), by the inflation-restriction sequence for $(\mathbf{P}_0, \mathbf{P}_0, \rho_{\mathbf{P}_0}; \{1, -1\}_1)$, and since $H^2(\bar{V}, \{1, -1\}_1) \approx C_2$, we obtain

$$H_b^2(\mathbf{P}', \{1, -1\}_1) \approx C_2 \times C_2.$$

Hence, together with the cohomology class of the trivial 2-cocycle and that of $\bar{\mu}^{(1)} = \bar{\mu}$, there exist two other elements of $H_b^2(\mathbf{P}', \{1, -1\}_1)$ having as representatives the 2-cocycles $\bar{\mu}^{(2)}$ and $\bar{\mu}^{(3)}$ defined by

$$\begin{aligned} \bar{\mu}^{(2)}((t, \Lambda v), (t', \Lambda' v')) &= \begin{cases} -\bar{\mu}^{(1)}((t, \Lambda v), (t', \Lambda' v')) & \text{if } v = v' = \bar{e}, \\ \bar{\mu}^{(1)}((t, \Lambda v), (t', \Lambda' v')) & \text{otherwise,} \end{cases} \\ \bar{\mu}^{(3)}((t, \Lambda v), (t', \Lambda' v')) &= \begin{cases} -1 & \text{if } v = v' = \bar{e}, \\ 1 & \text{otherwise} \end{cases} \end{aligned}$$

for all $(t, \Lambda), (t', \Lambda')$ in \mathbf{P}_0 and all v, v' in \bar{V} . As $H_c^1(\mathbf{P}', \mathbf{U}(1)_1) \approx C_2$, we prove that the group

$$\bar{\mathbf{P}}'^{(2)} = \{1, -1\}_1 \bar{\mu}^{(2)} \mathbf{P}'$$

(equipped with an obvious group topology) is a quantum mechanical \mathbf{P}' -group by showing that (Ref. 1, Corollary to Proposition B.1)

$$H_c^1(\bar{\mathbf{P}}'^{(2)}, \mathbf{U}(1)_1) \approx C_2. \quad (\text{III. 1})$$

If $f \in Z_c^1(\bar{\mathbf{P}}'^{(2)}, \mathbf{U}(1)_1)$, we have

$$f(\xi, (t, \Lambda)) = 1 \quad (\text{III. 2})$$

for all $\xi \in \{1, -1\}$ and all $(t, \Lambda) \in \mathbf{P}_0$. For, if we put $\bar{\mu}^{(2)}|_{\mathbf{P}_0 \times \mathbf{P}_0} = \bar{\mu}^{(2)}$, the subgroup $\{1, -1\}_1 \bar{\mu}^{(2)} \mathbf{P}_0$ of $\bar{\mathbf{P}}'^{(2)}$ is topologically isomorphic to $\mathbf{ISL}(2, \mathbf{C})$. Furthermore,

$$\begin{aligned} f(1, \bar{e}) &= f(\xi, (t, \Lambda)) f(1, \bar{e}) = f(\xi, (t, \Lambda \bar{e})) \\ &= f(-\xi, (t, \Lambda)) f(-1, \bar{e}) = f(-1, \bar{e}) \end{aligned} \quad (\text{III. 3})$$

for all $\xi \in \{1, -1\}$ and all $(t, \Lambda) \in \mathbf{P}_0$. On the other hand, since $f(1, \bar{e})^4 = 1$, $f(1, \bar{e}) \in \{\pm i, \pm 1\}$; yet it follows from (III. 3) that actually $f(1, \bar{e}) \in \{1, -1\}$, hence (III. 1) is satisfied and $\bar{\mathbf{P}}'^{(2)}$ is a quantum mechanical \mathbf{P}' -group which is not topologically isomorphic to $\bar{\mathbf{P}}'^{(1)}$. If $E^{(3)}$ denotes the topological group $\{1, -1\}_1 \bar{\mu}^{(3)} \mathbf{P}'$, we have that $H_c^1(E^{(3)}, \mathbf{U}(1)_1)$ is a cyclic group of order 4 because relation (III. 2) [and then (III. 3)] is not satisfied by $f \in Z_c^1(E^{(3)}, \mathbf{U}(1)_1)$. Therefore, up to topological group isomorphisms, we have only two different quantum mechanical \mathbf{P}' -groups, namely, $\bar{\mathbf{P}}'^{(1)}$ and $\bar{\mathbf{P}}'^{(2)}$.

(A. 3) \mathbf{P}_* : Since $Z_c^1(\mathbf{P}_*, \mathbf{U}(1)_{\Phi_{\mathbf{P}_0}}) \approx \mathbf{U}(1)$, the representation group

$$\bar{\mathbf{P}}_* = \{1, -1\}_1^2 \bar{\mu}' \mathbf{P}_*$$

for $(\mathbf{P}_*, \mathbf{P}_0)$ is unique up to topological group isomorphisms (Proposition B), i. e., it is THE quantum mechanical \mathbf{P}_* -group. The mapping

$$((\xi, \xi'), (t, \Lambda v)) \mapsto (\xi', ((t, \xi\sigma(\Lambda)), v)) \quad (\text{III. 4})$$

$$(\xi, \xi' \text{ in } \{1, -1\}; (t, \Lambda) \in \mathbf{P}_0; v \in \bar{V}')$$

is a topological group isomorphism

$$\bar{\mathbf{P}}_* \rightarrow \{1, -1\}_1 \bar{V}' (\mathbf{ISL}(2, \mathbf{C}) \times_{\bar{v}'} \bar{V}'),$$

where \bar{v}' is defined by

$$\begin{aligned} \bar{v}'((t, A), v), ((t', A'), v')) &= \bar{\mu}'_2((t, \rho_{\mathbf{L}_0}(A)v), (t', \rho_{\mathbf{L}_0}(A')v')). \end{aligned} \quad (\text{III. 5})$$

(A. 4) \mathbf{P}'_* : Also in this case we have

$$Z_c^1(\mathbf{P}'_*, \mathbf{U}(1)_{\Phi_{\mathbf{P}_0}}) \approx \mathbf{U}(1),$$

so that the representation group

$$\bar{\mathbf{P}}'_* = \{1, -1\}_1^2 \mu' \mathbf{P}'_*$$

for $(\mathbf{P}'_*, \mathbf{P}_0)$ can be called THE quantum mechanical \mathbf{P}'_* -group (being unique up to topological group isomorphisms). Here, the mapping (III. 4) with $v \in V'$ is a topological group isomorphism

$$\bar{\mathbf{P}}'_* \rightarrow \{1, -1\}_1 \nu' (\mathbf{ISL}(2, \mathbf{C}) \times_{\nu'} V'),$$

where ν' is defined by (III. 5) with ν' instead of \bar{v}' and μ'_2 instead of $\bar{\mu}'_2$.

(A. 5) \mathbf{P} : The topological group

$$\bar{\mathbf{P}}^{(1)} = \{1, -1\}_1^3 \mu \mathbf{P}$$

is a representation group for $(\mathbf{P}, \mathbf{P}')$, i. e., a quantum mechanical \mathbf{P} -group, and the mapping

$$\begin{aligned} ((\xi, \xi', \xi''), (t, \Lambda v)) &\mapsto ((\xi', \xi''), ((t, \xi\sigma(\Lambda)), v)) \\ &(\xi, \xi', \xi'' \text{ in } \{1, -1\}; (t, \Lambda) \in \mathbf{P}_0; v \in V) \end{aligned}$$

is a topological group isomorphism

$$\bar{\mathbf{P}}^{(1)} \rightarrow \{1, -1\}_1^2 \nu (\mathbf{ISL}(2, \mathbf{C}) \times_{\nu} V),$$

where ν is defined by

$$\begin{aligned} \nu((t, A), v), ((t', A'), v')) &= (\mu_2((t, \rho_{\mathbf{L}_0}(A)v), (t', \rho_{\mathbf{L}_0}(A')v')), \\ &\mu_3((t, \rho_{\mathbf{L}_0}(A)v), (t', \rho_{\mathbf{L}_0}(A')v'))). \end{aligned}$$

However, $\bar{\mathbf{P}}^{(1)}$ is not the unique representation group for $(\mathbf{P}, \mathbf{P}')$ (up to topological group isomorphisms). To prove this, we first consider the "possible" non-Abelian representation groups for (V, \bar{V}) . They are the non-Abelian groups of order 16 whose centers contain a subgroup isomorphic to V . In Table I we give, by generators and relations, a representative F_i ($1 \leq i \leq 9$) for each of the nine classes of isomorphic non-Abelian groups of order 16 (cf. Ref. 13, Sec. 118). The neutral elements of the F_i are all denoted by e . The meaning of $\langle \odot \rangle$ in Table I is that of the subgroup generated by \odot ; D_m denotes a dihedral group of order $2m$, Q_n a generalized quaternion group of order $4n$, and qD_m a quasi-dihedral group of order $2m$ (Ref. 14, Kap. I, 14.9). It follows that only the groups F_i for $2 \leq i \leq 5$ are "possible" non-Abelian representation groups for (V, \bar{V}) . On the other hand, if F_i is such a representation group, there are *a priori* three admissible splitting projections $\rho_{i,j}$ ($1 \leq j \leq 3$) of F_i onto V up to the interchange of e' and \bar{e}' . Furthermore, since

$$\hat{V} \approx V \approx H^2(V, \mathbf{U}(1)_{\Phi_{\bar{V}}}),$$

it is enough that F_i satisfies, for at least one j ,

TABLE I. The non-Abelian groups of order 16.

Symbol	Set of generators	Relations	Center
F_1	$\{a, b, c\}$	$a^4 = e, b^2 = e, c^2 = e, cbc^{-1} = ba^2, bab^{-1} = a, cac^{-1} = a$	$\langle a \rangle$
F_2	$\{a, b, c\}$	$a^4 = e, b^2 = e, c^2 = e, cac^{-1} = ab, cbc^{-1} = b, bab^{-1} = a$	$\langle a^2, b \rangle$
F_3	$\{a, b, c\}$	$a^4 = e, b^2 = e, c^2 = e, cac^{-1} = a^{-1}, cbc^{-1} = b, bab^{-1} = a$	$\langle a^2, b \rangle$
F_4	$\{a, b, c\}$	$a^4 = e, a^2 = b^2, c^2 = e, cac^{-1} = a, cbc^{-1} = b, bab^{-1} = a^{-1}$	$\langle a^2, c \rangle$
F_5	$\{a, b\}$	$a^4 = e, b^4 = e, bab^{-1} = a^{-1}$	$\langle a^2, b^2 \rangle$
F_6	$\{a, b\}$	$a^8 = e, b^2 = e, bab^{-1} = a^{-3}$	$\langle a^2 \rangle$
$F_7 = D_8$	$\{a, b\}$	$a^8 = e, b^2 = e, bab^{-1} = a^{-1}$	$\langle a^4 \rangle$
$F_8 = qD_8$	$\{a, b\}$	$a^8 = e, b^2 = e, bab^{-1} = a^3$	$\langle a^4 \rangle$
$F_9 = Q_4$	$\{a, b\}$	$a^8 = e, a^4 = b^2, bab^{-1} = a^{-1}$	$\langle a^4 \rangle$

$$H^1(F_i, U(1)_{\Phi_{N_{i,j}}}) \approx H^1(V, U(1)_{\Phi_{\bar{V}}}) \approx C_2,$$

where $N_{i,j} = \rho_{i,j}^{-1}(\bar{V})$ (Ref. 1, Corollary to Proposition B.1). The groups $N_{i,j}$ and $H^1(F_i, U(1)_{\Phi_{N_{i,j}}})$ ($2 \leq i \leq 5; 1 \leq j \leq 3$) are given in Table II. It follows from this table that every non-Abelian representation group for (V, \bar{V}) is isomorphic to F_2 with splitting projection $\rho_{2,2}$ or to F_5 with splitting projection $\rho_{5,2}$ or $\rho_{5,3}$. We have topological operations $\Psi_i = \varphi \circ \rho_{i,2}$ ($i = 2, 5$) of F_i on $ISL(2, C)$, where φ is as above. Then the topological semidirect products

$$E_i(\mathbf{P}) = ISL(2, C) \times_{\Psi_i} F_i \quad (i = 2, 5)$$

are nonisomorphic representation groups for $(\mathbf{P}, \mathbf{P}')$ with splitting projections

$$\rho_i : ((t, A), d) \mapsto (\rho_{\mathbf{P}_0}(t, A), \rho_{i,2}(d))$$

because

$$H_c^1(E_i(\mathbf{P}), U(1)_{\Phi_{\mathbf{P}' \circ \rho_i}}) \approx H_c^1(\mathbf{P}, U(1)_{\Phi_{\mathbf{P}'}}) \approx C_2.$$

On the other hand, if $\Psi_5^{(2)} = \varphi \circ \rho_{5,3}$,

$$E_5^{(2)}(\mathbf{P}) = ISL(2, C) \times_{\Psi_5^{(2)}} F_5,$$

and ι is the automorphism of F_5 defined by $\iota(a) = a$ [or $\iota(ab) = b$], $\iota(b) = ab$ (with the generators a, b given in Table I), then the mapping

$$((t, A), d) \mapsto ((t, A), \iota(d)) \quad ((t, A) \in ISL(2, C); d \in F_5)$$

is a topological group isomorphism of $E_5(\mathbf{P})$ onto $E_5^{(2)}(\mathbf{P})$. Moreover, there exists a topological group isomorphism of $E_2(\mathbf{P})$ onto $\bar{\mathbf{P}}^{(4)}$ defined by

$$((t, \xi\sigma(\Lambda)), d) \mapsto ((\xi, \xi'_d, \xi''_d), (t, \Lambda v_d)) \quad (\xi \in \{1, -1\}; (t, \Lambda) \in \mathbf{P}_0; d \in F_2),$$

where, if a, b, c are the generators of F_2 given in Table I,

$$\xi'_a = \xi''_a = \xi'_c = \xi''_c = -\xi'_b = -\xi''_b = 1$$

and

$$v_a = e' \quad (\text{or } v_a = \bar{e}'), \quad v_b = e, \quad v_c = \bar{e}.$$

TABLE II. The cohomology groups $H^1(F_i, U(1)_{\Phi_{N_{i,j}}})$ ($2 \leq i \leq 5$).

F_i	$N_{i,j}$	$H^1(F_i, U(1)_{\Phi_{N_{i,j}}}) \approx$
F_2	$N_{2,1} = \langle a, b \rangle$	C_4
	$N_{2,2} = \langle a^2, b, c \rangle$	C_2
	$N_{2,3} = \langle ac, a^2, b \rangle$	$C_4 \times C_2$
F_3	$N_{3,1} = \langle a, b \rangle$	$C_4 \times C_2$
	$N_{3,2} = \langle a^2, b, c \rangle$	$C_2 \times C_2$
	$N_{3,3} = \langle ac, a^2, b \rangle$	$C_2 \times C_2$
F_4	$N_{4,1} = \langle a, c \rangle$	$C_2 \times C_2$
	$N_{4,2} = \langle b, c \rangle$	$C_2 \times C_2$
	$N_{4,3} = \langle ab, a^2, c \rangle$	$C_2 \times C_2$
F_5	$N_{5,1} = \langle a, b^2 \rangle$	C_4
	$N_{5,2} = \langle a^2, b \rangle$	C_2
	$N_{5,3} = \langle ab, a^2, b^2 \rangle$	C_2

Proceeding as above, it is easy to check that among the five classes of isomorphic Abelian groups of order 16 there is only one class of (isomorphic) representation groups for (V, \bar{V}) . A representative of this class is the group $F_0 = C_4 \times C_4$ defined by generators a, b and relations $a^4 = e, b^4 = e, bab^{-1} = a$. A splitting projection ρ'_0 of F_0 onto V can be defined by $\rho'_0(a) = \bar{e}$ and $\rho'_0(b) = e'$. If Ψ_0 denotes the topological operation $\varphi \circ \rho'_0$ of F_0 on $ISL(2, C)$, the topological semidirect product

$$E_0(\mathbf{P}) = ISL(2, C) \times_{\Psi_0} F_0$$

is a representation group for $(\mathbf{P}, \mathbf{P}')$ with splitting projection $\rho_0 : ((t, A), d) \mapsto (\rho_{\mathbf{P}_0}(t, A), \rho'_0(d))$ (cf. Ref. 18, Secs. 2 and 3), and it is not isomorphic to $E_2(\mathbf{P})$ or $E_5(\mathbf{P})$. The interchange, in the definition of ρ'_0 , of a, b in F_0 or of e', \bar{e}' in V will lead to representation groups for $(\mathbf{P}, \mathbf{P}')$ which are topologically isomorphic to $E_0(\mathbf{P})$.

Remark 1: In order to find the CUAP-reps of \mathbf{P} , it is common practice^{6,7} to study the CUAP-reps of $ISL(2, C) \times_{\varphi} V$. This *a priori* arbitrary procedure is justified by the result of (A. 5).

Remark 2: By removing all translations in Sec. II A, we obtain the corresponding results for $L_0, L', L_+, L'_+,$ and L .

B. The Galilei groups

The role of $ISL(2, C)$ is played here by the universal covering group \bar{G}_0 of G_0 and we make the usual identification of each element g of \bar{G}_0 with a 4-tuple $(t_g^0, \mathbf{t}_g, \mathbf{v}_g, A_g)$, where $t_g^0, \mathbf{t}_g, \mathbf{v}_g$ are as in the case of G_0 and $A_g \in SU(2, C)$. The results for the quantum mechanical Galilei groups are analogous, *mutatis mutandis*, to those for the Poincaré groups and are given in Table III. There, φ is the topological operation of V on G_0 such that, for each $g \in \bar{G}_0$,

$$\varphi(\bar{e})(t_g^0, \mathbf{t}_g, \mathbf{v}_g, A_g) = (t_g^0, -\mathbf{t}_g, -\mathbf{v}_g, A_g),$$

$$\varphi(e')(t_g^0, \mathbf{t}_g, \mathbf{v}_g, A_g) = (-t_g^0, \mathbf{t}_g, -\mathbf{v}_g, A_g).$$

The meaning of $\bar{\varphi}, \varphi', \bar{\varphi}'$ and of $\xi_0, \bar{\xi}, \dots, \nu', \nu$ should be clear. In addition, we have the topological operations Ψ_i ($i = 2, 5, 0$) of F_i on \bar{G}_0 defined by $\Psi_i = (\varphi_{N_{i,2}}, \varphi \circ \rho_{i,2})$ for $i = 2, 5$ and by $\Psi_0 = (\varphi_{N_0}, \varphi \circ \rho'_0)$, where $N_0 = \rho_0^{-1}(\bar{V})$. The topological group isomorphisms of Table III are obtained from the corresponding ones

TABLE III. The quantum mechanical Galilei groups \bar{G} .

(G, N)	\bar{G}	$Z_c^1(G, U(1)_{\Phi_N}) \approx$
G_0	$\bar{G}_0 = (\mathbf{R} \times \{1, -1\})_1(\eta_0, \mu_0)G_0$ $\cong \mathbf{R}_1 \zeta_0 \tilde{G}_0$	\mathbf{R}
G'	$\bar{G}'^{(1)} = (\mathbf{R} \times \{1, -1\})_1(\bar{\eta}, \bar{\mu}^{(1)})G'$ $\cong \mathbf{R}_1 \bar{\zeta}(\tilde{G}_0 \times \bar{v})$ $\bar{G}'^{(2)} = (\mathbf{R} \times \{1, -1\})_1(\bar{\eta}, \bar{\mu}^{(2)})G'$	$\mathbf{R} \times C_2$
(G_+, G_0)	$\bar{G}_+ = (\mathbf{R} \times \{1, -1\}^2)_{\circ} G_0(\bar{\eta}', \bar{\mu}')G_+$ $\cong (\mathbf{R} \times \{1, -1\})_{\circ} \tilde{G}_0(\bar{\zeta}', \bar{\nu}')(\tilde{G}_0 \times \bar{v}, \bar{v}')$	$\mathbf{R} \times U(1)$
(G_{++}^+, G_0)	$\bar{G}_{++}^+ = (\mathbf{R} \times \{1, -1\}^2)_{\circ} G_0(\eta', \mu')G_{++}^+$ $\cong (\mathbf{R} \times \{1, -1\})_{\circ} \tilde{G}_0(\zeta', \nu')(\tilde{G}_0 \times \bar{v}, \bar{v}')$	$\mathbf{R} \times U(1)$
(G, G')	$\bar{G}^{(1)} = (\mathbf{R} \times \{1, -1\}^3)_{\circ} G'(\eta, \mu)G$ $\cong (\mathbf{R} \times \{1, -1\}^2)_{\circ} M(\zeta, \nu)(\tilde{G}_0 \times \bar{v})$ where $M = \tilde{G}_0 \times \bar{v}$ $\cong E_2(G) = \bar{G}_0 \times \psi_2 F_2$ $E_3(G) = \bar{G}_0 \times \psi_3 F_3$ $E_0(G) = \bar{G}_0 \times \psi_0 F_0$	$\mathbf{R} \times U(1) \times C_2$

for the Poincaré groups by replacing $(t, \Lambda) \in P_0$ with $g \in G_0$ and by "adding the reals." If $(G, N) \in \{G_0, (G_+, G_0), (G_{++}^+, G_0)\}$, the group \bar{G} is the unique second countable locally compact representation group for (G, N) up to topological group isomorphisms: It is THE quantum mechanical G -group. This assertion follows from Proposition B. If $G = G'$, we have, using Ref. 11, Corollary to Theorem 1 and then proceeding as in the case of P^1 ,

$$H_b^2(G', (\mathbf{R} \times C_2)_1) \approx H_b^2(G', \mathbf{R}_1) \times H_b^2(G', (C_2)_1) \approx \mathbf{R} \times C_2 \times C_2.$$

Up to topological group isomorphisms, there exist only two different quantum mechanical G' -groups, namely, $\bar{G}'^{(1)}$ and $\bar{G}'^{(2)}$. In fact, "adding the reals" does not increase the number of classes of isomorphic quantum mechanical G' -groups (in analogy with the case of G_0).

APPENDIX A

The following proposition is a corollary to Ref. 11, Proposition 1.

Proposition A: Let G be a Polish group which is the topological semidirect product of a subgroup S by a subgroup K and let A_ψ be a Polish G -module such that $\Psi(K) = \{\text{Id}_A\}$. Then

$$H_b^2(G, A_\psi) \approx H_b^2(K, A_1)^S \times H_b^2(S, A_\psi|_S)$$

in each of the following two cases:

- $Z_c^1(K, A_1)$ is trivial,
- S is finite and $Z_c^1(K, A_1)$ is divisible and torsion free.

Proof: We begin with an observation valid in both cases. The notation and results of Ref. 11, Proposition 1 and of the remark preceding it, yet with the groups written multiplicatively, are tacitly understood (cf. Ref. 15, Remark 1).

If $[f_1] \in H_b^2(K, A_1)^S$, there exists, for each $s \in S$, an element $f_2^{(s)}$ of $C_b^1(K, A_1)$ satisfying $\Psi_2^1(s)f_1 = f_1 \delta f_2^{(s)}$. Moreover, we can choose $f_2^{(e^s)}$ satisfying $f_2^{(e^s)}(k) = e_A$ for all $k \in K$. It follows that

$$f_2^{(s)}(\hat{\Psi}^1(s)f_2^{(s')})(f_2^{(ss')})^{-1} = h_{(s, s')} \in Z_c^1(K, A_1) \quad (A)$$

for all s, s' in S and we check that the mapping $h : (s, s') \mapsto h_{(s, s')}$ belongs to $Z^2(S, Z_c^1(K, A_1)_{\hat{\Psi}_2^1|_S})$.

Now in case (a) we have $H_b^2(K, A_1)' = H_b^2(K, A_1)^S$, whence the assertion, because condition (ii') is satisfied by virtue of (A). In case (b), $H^2(S, Z_c^1(K, A_1)_{\hat{\Psi}_2^1|_S})$ is trivial by Ref. 12, Chap. IV, Corollary 5.4. Hence there exists $l \in C^1(S, Z_c^1(K, A_1)_{\hat{\Psi}_2^1|_S})$ such that

$$h(s, s') = l(s)(\hat{\Psi}_2^1(s)l(s'))l(ss')^{-1}$$

for all s, s' in S , where h is as above. We have $H_b^2(K, A_1)' = H_b^2(K, A_1)^S$ because (i') and (ii') are satisfied by f_1 and $f_2^{(s)} = f_2^{(s')}l(s)^{-1}$ ($s \in S$). Indeed, if f_2 is given by Ref. 11, (4.5), the mapping $f_2' : K \times S \rightarrow A$ defined by

$$f_2'(k, s) = f_2(k, s)(\Psi(s)l(s^{-1})(k))$$

is Borel (by Ref. 16, Sec. 31, V, Theorem 2) and we have

$$f_2'^{(s)}(k) = \Psi(s)f_2'(k, s^{-1})^{-1}$$

for all $s \in S$ and all $k \in K$. ■

Remark: If the Abelian group A is divisible and torsion free, then so is $Z_c^1(K, A_1)$ (Ref. 11, proof of Proposition 2). It follows that case (b) of Proposition A improves Ref. 11, Proposition 2.

APPENDIX B

Proposition B: Let G be a second countable locally compact group and let N be a closed normal subgroup of G of index 1 or 2. Suppose that the following conditions are satisfied:

- $H_B^2(G, \mathbf{R}_{\Phi_N})$ is isomorphic to the additive group of \mathbf{R}^n ($n \geq 0$).
- Let π be the covering projection of \mathbf{R} onto $U(1)$. The group homomorphism $(\tilde{\pi}_B)_*$ of $H_B^2(G, \mathbf{R}_{\Phi_N})$ into $H_B^2(G, U(1)_{\Phi_N})$ has closed kernel in the canonical topology and countable cokernel.
- $Z_c^1(G, U(1)_{\Phi_N})$ is divisible.

Then, if E, E' are two arbitrary representation groups for (G, N) with, respectively, splitting projections ρ, ρ' , there exists a topological group isomorphism λ of E' onto E such that $\rho \circ \lambda = \rho'$.

Proof: We generalize an argument of Moore (Ref. 17, Proposition 3.2) and use the notation of Ref. 1, Proposition 8. Take the $(G, N)_B$ -selector s and the representation group $s(H_B^2)_{\Phi_N}^* \text{ev}^* G$ for (G, N) with splitting projection pr_2 considered in Ref. 1, Corollary to Proposition 5. If σ is the Borel splitting section $g \mapsto (e_s(H_B^2), g)$, then $s = s_\sigma$ (Ref. 1, Remark 6). We

identify E (resp. E') with $s_\sigma(H_B^2) \circ_{\phi_N} fG$ [resp. with $s_\sigma(H_B^2) \circ_{\phi_N} f'G$] by means of κ_σ^E (resp. of $\kappa_\sigma^{E'}$), where f (resp. f') is in $Z_b^2(G, s_\sigma(H_B^2) \circ_{\phi_N})$, and choose a normalized Borel section σ_1 (resp. σ_2) associated with ρ (resp. with ρ'). For each $[\mu] \in H_B^2(G, U(1)_{\phi_N})$, we put

$$s_{\sigma_2}([\mu])^{-1} s_{\sigma_1}([\mu]) = [\mu]_{(\sigma_1, \sigma_2)}$$

and see that $[\mu]_{(\sigma_1, \sigma_2)} \in B_b^2(G, U(1)_{\phi_N})$. On the other hand, the extension $(C_b^1(G, U(1)_{\phi_N}), \delta)$ of $B_b^2(G, U(1)_{\phi_N})$ by $Z_c^1(G, U(1)_{\phi_N})$ is inessential by virtue of assumption (3), and so there exists an injective group homomorphism

$$\beta : B_b^2(G, U(1)_{\phi_N}) \rightarrow C_b^1(G, U(1)_{\phi_N})$$

such that $\delta(\beta(\mu)) = \mu$ for all $\mu \in B_b^2(G, U(1)_{\phi_N})$. We then have an element h of $C_b^1(G, s_\sigma(H_B^2) \circ_{\phi_N})$ defined by

$$h(g)(s_\sigma([\mu])) = \beta([\mu]_{(\sigma_1, \sigma_2)})(g) \quad ([\mu] \in H_B^2(G, U(1)_{\phi_N})).$$

Indeed, $h(g)$ is a group homomorphism for all $g \in G$ because so are s_σ , s_{σ_1} , s_{σ_2} , and β . Furthermore, if $[\mu]$ is given by Ref. 1, (III, 3), we have

$$[\mu]_{(\sigma_1, \sigma_2)} = \left(\prod_{i=1}^n (i_{\sigma\sigma_2}(\pi \circ r_i \nu_i)^{-1} i_{\sigma\sigma_1}(\pi \circ r_i \nu_i)) \right) i_{\sigma\sigma_2}(s''([\epsilon]))^{-1} i_{\sigma\sigma_1}(s''([\epsilon])) \quad (r_i \in \mathbf{R}),$$

whence the continuity of $h(g)$ for all $g \in G$, with an appropriate choice of β . Since the mapping $g \mapsto h(g) \times (S_\sigma([\mu]))$ of G into $U(1)$ is Borel for all $[\mu] \in H_B^2(G, U(1)_{\phi_N})$, h is Borel by the argument at the beginning of the proof of Ref. 1, Proposition 5; therefore, $h \in C_b^1(G, s_\sigma(H_B^2) \circ_{\phi_N})$. To end our proof, it is enough to remark that

$$\begin{aligned} (f'(g, g')^{-1} f(g, g'))(s_\sigma([\mu])) &= [\mu]_{(\sigma_1, \sigma_2)}(g, g') \\ &= \delta(\beta([\mu]_{(\sigma_1, \sigma_2)}))(g, g') \\ &= (\delta h(g, g'))(s_\sigma([\mu])) \end{aligned}$$

for all g, g' in G and all $[\mu] \in H_B^2(G, U(1)_{\phi_N})$ because we can choose

$$f'^{-1} f = (\hat{i}_{\sigma\sigma_2} \circ \text{ev}^{\sigma_2})^{-1} (\hat{i}_{\sigma\sigma_1} \circ \text{ev}^{\sigma_1}).$$

As usual, we have denoted two different coboundary operators by the same symbol δ . ■

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Some classes of exact solutions of the nonlinear Boltzmann equation^{a)}

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We derive and discuss some exact solutions of the full (nonlinear) Boltzmann equation. One of these is the similarity solution recently found by Krook and Wu for the velocity relaxation problem. Other similarity solutions do exist, and we point out their usefulness in the search for exact solutions of the spatially inhomogeneous Boltzmann equation.

I. INTRODUCTION

In a recent paper Krook and Wu¹ reported an interesting exact solution of the full (nonlinear) Boltzmann equation, describing the relaxation of the distribution function to the equilibrium Maxwellian. They considered an infinite, spatially homogeneous and isotropic monatomic gas, with a model potential such that the elastic differential cross section is given by

$$\sigma(g, \chi) = \kappa/g, \quad (1.1)$$

where κ is a constant, g is the relative speed, and χ the scattering angle in the center of mass system.

The work of Krook and Wu is remarkable for several reasons. First, of course, is the fact that they obtained an exact solution to the relaxation problem, and exact solutions of the Boltzmann equation are hard to come by. As is well known, the only exact solutions that were previously available consists of very special local Maxwellians, namely those such that the fluid dynamical variables are solutions of the Euler equation which satisfy the condition that the heat flux vector and the stress tensor vanish, and therefore are simultaneously solutions of the Navier-Stokes equations.² These solutions are not particularly interesting, since a local Maxwellian makes the collision integral vanish identically, and one cannot therefore obtain information about dissipative processes.

There is a second important aspect to the work of Krook and Wu. By using an ingenious method, they transformed the original nonlinear integrodifferential equation into a nonlinear partial differential equation, for which they wrote down a similarity solution of the "shock transition" type, without however giving a derivation. Because there exist well established group-theoretic methods of searching for similarity solutions of differential equations,³ it seems of interest to carry the analysis of Krook and Wu a step further, and explore whether other similarity solutions exist for the full Boltzmann equation, and if so, for what problems of rarefied gas dynamics they might be relevant.

It is the object of this paper to report on such an analysis. In the next section we shall first review briefly the method of Krook and Wu. This will serve us to indicate the few cases in which our notation differs and, at the same time, to point out a minor aspect of their derivation which is incorrect.

II. THE KROOK-WU SIMILARITY SOLUTION

The state of the gas at time t is described by the distribution function $nf(t, v)$, where n is the constant number density and $v = |v|$ is the speed of a particle. Since the system is spatially homogeneous, and assuming that the cross section is given by (1.1), the Boltzmann equation becomes⁽¹⁾:

$$\begin{aligned} \frac{\partial}{\partial \tau} f(\tau, v) & \\ &= -f(\tau, v) + \frac{1}{4\pi} \int dw \int_0^\pi d\chi \sin \chi \int_0^{2\pi} d\epsilon f(\tau, v') f(t, w'). \end{aligned} \quad (2.1)$$

Here, as usual, the primed variables refer to the speeds after collision, whose relation to v, w, χ and ϵ is given by Eqs. (6) and (7) of Ref. 1; $\tau = 4\pi n \kappa t$ is a dimensionless time variable, and the condition of constant density

$$\int dv f(\tau, v) = 1 \quad (2.2)$$

has been used. Of course the kinetic energy is a constant as well, so that

$$\int dv v^2 f(\tau, v) = 3 (k_B T/m) \equiv 3\beta^2, \quad (2.3)$$

where k_B is Boltzmann's constant, m is the mass and T the constant temperature.

The central idea of the Krook-Wu method is the following. Defining normalized moments of $f(\tau, v)$ by

$$M_n(\tau) = \frac{\pi^{1/2}}{2(2\beta^2)^n \Gamma(n + \frac{3}{2})} \int dv v^{2n} f(\tau, v) \quad (n=0, 1, 2, \dots) \quad (2.4)$$

allows a transformation of (2.1) into the following ordinary differential equation (o.d.e.):

$$\frac{d}{d\tau} M_n(\tau) + M_n(\tau) = \frac{1}{n+1} \sum_{m=0}^n M_m(\tau) M_{n-m}(\tau). \quad (2.5)$$

Furthermore, introducing a generating function for the moments

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$$G(\tau, \xi) = \sum_{n=0}^{\infty} \xi^n M_n(\tau), \quad (2.6)$$

and making subsequently the transformation of variables

$$x = (1 - \xi)/\xi \quad u(\tau, x) = \xi^{-1} G(\tau, \xi), \quad (2.7)$$

allows a reduction of the o. d. e. (2.5) to the following partial differential equation (p. d. e.)

$$u_{x\tau} + u_x + u^2 = 0. \quad (2.8)$$

where the subscripts x and τ stand for partial differentiation.

At this point Krook and Wu notice that (2.8) admits the similarity solution

$$u(\tau, x) = x^{-1} F(\eta), \quad \eta = \ln x + c\tau, \quad (2.9)$$

where c is a constant still to be determined. This is done by imposing the conditions

$$M_0(\tau) = M_1(\tau) = 1, \quad (2.10)$$

which correspond to equations (2.2) and (2.3). Thus one finds $c = \frac{1}{6}$. Then substitution of (2.9) into (2.8) gives

$$F'' + 5F' - 6F(1 - F) = 0, \quad (2.11)$$

where the primes denote differentiation with respect to the similarity variable η . Equation (2.11) can be reduced to a first order o. d. e., i. e.,

$$p p' + 5p - 6F(1 - F) = 0 \quad (2.12)$$

in terms of the variable $p = p(F) = dF/d\eta$. And the solution of (2.12) is

$$p = 2(1 - F)(1 - \sqrt{1 - F}), \quad (2.13)$$

which, in turn, gives

$$F(\eta) = 1 - (1 + \exp\{\eta + b\})^{-2}, \quad (2.14)$$

where b is a constant to be determined.

With the explicit expression (2.14) for $F(\eta)$ the function $u(\tau, x)$ is known, and so is $G(\tau, \xi)$. Therefore, the moments $M_n(\tau)$ can be determined, after which an inversion of (2.4) gives the distribution function $f(\tau, v)$. The result is

$$f(\theta, v) = \frac{\exp(-v^2/2\beta^2\theta)}{2(2\pi\beta^2\theta)^{3/2}} \left[\frac{1}{\theta} (5\theta - 3) + \frac{1}{\theta^2} (1 - \theta) \left(\frac{v}{\beta} \right)^2 \right], \quad (2.15)$$

where the new time variable θ is defined by

$$\theta = 1 - \exp\left\{-\frac{1}{6}(\tau + \tau_0)\right\}, \quad (b = \tau_0/6). \quad (2.16)$$

The expression (2.15) is the same as the result of Krook and Wu, except for the definition of the new time variable, due to the presence of the constant τ_0 . This is necessary, of course, since the distribution function must be time-translationally invariant, as is easily seen from (2.1). The actual value of τ_0 —i. e., of the arbitrary constant of integration b in (2.14)—is determined by the requirement that

$$f(\tau, v) \geq 0 \quad (0 \leq \tau < \infty), \quad (2.17)$$

which gives $\tau_0 \geq -6 \ln \frac{2}{3} \cong 5.5$.

A second remark concerning the Krook-Wu solution

concerns the role played by the boundary conditions. In connection with the determination of the constant c appearing in the similarity variable η , they state that one needs not only the conditions (2.10), but also the further condition

$$M_n(\infty) = 1, \quad n = 0, 1, 2, \dots, \quad (2.18)$$

which corresponds to the relaxation of $f(\tau, v)$ to the absolute Maxwellian

$$f(\tau = \infty, v) = \frac{\exp(-v^2/2\beta^2)}{(2\pi\beta^2)^{3/2}}. \quad (2.19)$$

This is actually incorrect, i. e., the conditions (2.10) are sufficient to determine c , as the following proof shows.

We have on the one hand

$$1 = M_0(\tau) = \lim_{\xi \rightarrow 0} G(\tau, \xi), \quad (2.20)$$

and therefore

$$\frac{1}{\xi} u\left(\tau, \frac{1-\xi}{\xi}\right) = 1 \quad (\text{as } \xi \rightarrow 0) \quad (2.21)$$

which can also be written in terms of the variable x

$$u(\tau, x) = \frac{1}{1+x} + O\left(\frac{1}{x^2}\right) \quad (x \text{ large}). \quad (2.22)$$

On the other hand the second part of (2.10) can be written

$$1 = M_1(\tau) = \lim_{\xi \rightarrow 0} \xi \frac{\partial}{\partial \xi} G(\tau, \xi) \quad (2.23)$$

and therefore, in terms of the variable x ,

$$(1+x)^3 u_x + (1+x)^2 u + 1 = 0 \quad (\text{as } x \rightarrow \infty). \quad (2.24)$$

Letting $v = 1 + x$ and solving (2.24) gives

$$u(v) = D/v + 1/v^2 \quad (\text{as } v \rightarrow \infty) \quad (2.25)$$

where the constant $D = 1$ in virtue of (2.22). This translates into a condition for $F(v)$, namely

$$F(v) = 1 - 1/v^2 \quad (\text{as } v \rightarrow \infty). \quad (2.26)$$

But as $v \rightarrow \infty$ (for some fixed τ) we can write $v \sim e^\eta$; hence (2.26) becomes

$$F(\eta) \sim 1 - \exp(-2\eta). \quad (2.27)$$

Substituting into the equation for $F(\eta)$, i. e.,

$$F'' + c^{-1}(1-c)F' - (F/c)(1-F) = 0,$$

and retaining only terms $O[\exp(-2\eta)]$ gives $c = \frac{1}{6}$.

QED. We shall discuss further the role played by the boundary conditions in the next section.

III. OTHER CLASSES OF SIMILARITY SOLUTIONS. ROLE OF THE BOUNDARY CONDITIONS

The similarity solution discussed in the previous section was not derived by Krook and Wu,¹ but simply written down. It seems therefore of interest to show that it can be derived by the same group-theoretical methods which have been so successful in problems of fluid dynamics—among others—over the recent past.³

We concentrate first on the question of finding similarity solutions for the nonlinear p. d. e.

$$u_{x\tau} + u_x + u^2 = 0, \quad (3.1)$$

without imposing any boundary conditions. Thus we replace (3.1) by a system of first order p. d. e.'s

$$u_x = w, \quad (3.2)$$

$$w_\tau + w + u^2 = 0, \quad (3.3)$$

where $w = w(\tau, x)$. Then, in order to construct the main group leaving Eqs. (3.2) and (3.3) invariant, we seek an operator³

$$X = \eta_1 \frac{\partial}{\partial \tau} + \eta_2 \frac{\partial}{\partial x} + \sigma_1 \frac{\partial}{\partial u} + \sigma_2 \frac{\partial}{\partial w}, \quad (3.4)$$

whose first extension we shall write

$$\tilde{X} = X + \zeta_p \frac{\partial}{\partial p} + \zeta_q \frac{\partial}{\partial q} + \zeta_r \frac{\partial}{\partial r} + \zeta_s \frac{\partial}{\partial s}, \quad (3.5)$$

where $p = u_\tau$; $q = u_x$; $r = w_\tau$; $s = w_x$, and the expressions for the additional coordinates which are needed in this case are

$$\begin{aligned} \zeta_q &= \left(\frac{\partial}{\partial x} + q \frac{\partial}{\partial u} + s \frac{\partial}{\partial w} \right) \sigma_1 - p \left(\frac{\partial}{\partial x} + q \frac{\partial}{\partial u} + s \frac{\partial}{\partial w} \right) \eta_1 \\ &\quad - q \left(\frac{\partial}{\partial x} + q \frac{\partial}{\partial u} + s \frac{\partial}{\partial w} \right) \eta_2, \end{aligned} \quad (3.6)$$

$$\begin{aligned} \zeta_r &= \left(\frac{\partial}{\partial \tau} + p \frac{\partial}{\partial u} + r \frac{\partial}{\partial w} \right) \sigma_2 - r \left(\frac{\partial}{\partial \tau} + p \frac{\partial}{\partial u} + r \frac{\partial}{\partial w} \right) \eta_1 \\ &\quad - s \left(\frac{\partial}{\partial \tau} + p \frac{\partial}{\partial u} + r \frac{\partial}{\partial w} \right) \eta_2. \end{aligned} \quad (3.7)$$

Equations (3.2) and (3.3) are now rewritten in terms of the variables p, q, r and s , yielding the following system:

$$S: \begin{cases} q = w, \\ r + w + u^2 = 0. \end{cases}$$

The conditions that the group leaves (3.2) and (3.3) invariant are $\tilde{X}(S) = 0$ on the manifold S . Hence

$$\zeta_q = \sigma_2, \quad (3.8)$$

$$\zeta_r + \sigma_2 + 2u\sigma_1 = 0, \quad (3.9)$$

from which, using (3.6) and (3.7) and eliminating q and r by means of S , the set of determining equations for the operator X is obtained. This gives

$$\eta_1 = \eta_1(\tau), \quad (3.10)$$

$$\eta_2 = \eta_2(x), \quad (3.11)$$

$$\sigma_2 = \frac{\partial \sigma_1}{\partial x} + w \frac{\partial \sigma_1}{\partial u} - w \eta_2'(x), \quad (3.12)$$

$$\sigma_2 + 2u\sigma_1 + \frac{\partial \sigma_2}{\partial \tau} - (u^2 + w) \frac{\partial \sigma_2}{\partial w} + (u^2 + w) \eta_1'(\tau) = 0, \quad (3.13)$$

where the prime denotes differentiation with respect to the argument of the function involved.

Equations (3.10) to (3.13) can be solved exactly, with the result that the expressions for the coordinates of the operator X are

$$\eta_1(\tau) = \beta - \alpha \exp(\tau), \quad (3.14)$$

$$\eta_2(x) = \gamma x + \delta, \quad (3.15)$$

$$\sigma_1(\tau, u) = [\alpha \exp(\tau) - \gamma]u, \quad (3.16)$$

$$\sigma_2(\tau, w) = [\alpha \exp(\tau) - 2\gamma]w, \quad (3.17)$$

where α, β, γ , and δ are arbitrary constants. Thus a one-parameter group depending on four arbitrary constants is obtained. In order to find the invariants we must solve

$$X(I) = 0, \quad (3.18)$$

that is, with the help of Eqs. (3.14) to (3.17),

$$\frac{d\tau}{\beta - \alpha \exp(\tau)} = \frac{dx}{\gamma x + \delta} = \frac{du}{[\alpha \exp(\tau) - \gamma]u} = \frac{dw}{[\alpha \exp(\tau) - 2\gamma]w}. \quad (3.19)$$

It is now easy to find particular cases of similarity solutions. For instance, on choosing $\alpha = \delta = 0$, $\beta \neq 0$, $\gamma \neq 0$, and letting $c = \gamma/\beta$, we obtain

$$u(\tau, x) = x^{-1}F(\eta), \quad (3.20)$$

where F is an arbitrary function of the similarity variable $\eta = \ln x + c\tau$. Eq. (3.20) is just the class of similarity solutions found by Krook and Wu¹ and discussed in Sec. II. In a similar fashion other classes of similarity solutions can be found. For example, letting $\alpha = \beta = \delta = 0$ and $\gamma \neq 0$ in (3.19) we obtain

$$u(\tau, x) = (\gamma x)^{-1}H(\tau), \quad (3.21)$$

where H is an arbitrary function of τ . Substitution of (3.21) in (3.1) gives the first order o. d. e.

$$H' + H - \gamma^{-1}H^2 = 0, \quad (3.22)$$

whose solution is

$$H(\tau) = [C \exp(\tau) + 1]^{-1} \quad (C = \text{arbitrary constant}) \quad (3.23)$$

so that (3.21) becomes

$$u(\tau, x) = (\gamma x)^{-1} [C \exp(\tau) + 1]^{-1}. \quad (3.24)$$

Naturally, whether a similarity solution of Eq. (3.1) is physically acceptable or not will depend on the specific boundary conditions that the problem under study imposes. And since the Krook-Wu procedure changes the order of the differential equations involved in the various stages of the calculation, obviously the proper number of boundary conditions changes too. In particular this can be easily seen in the velocity relaxation problem, where a solution of the spatially homogeneous Boltzmann equation is sought subject to the condition that the number density is constant at all times. Here the theorem proved by Carleman for hard-sphere potentials and by Morgenstern for pseudo-Maxwellian molecules (see, e. g., Ref. 4) can be invoked to conclude that such a problem has a unique solution, namely the Krook-Wu solution. On the other hand, while it is an easy matter to show that the condition $M_0(\tau) = 1$ implies that the condition

$$u(\tau, x = \infty) = 0 \quad (3.25)$$

holds for the variable $u(\tau, x)$, the converse is not true. For instance, the similarity solution (3.21) obviously satisfies (3.25). But the corresponding expression for the moments of the distribution function is

$$M_n(\tau) = \gamma^{-1} [1 + C \exp(\tau)]^{-1} \quad (\text{any } n), \quad (3.26)$$

in violation of the condition of constant density. In

other words we must impose a second boundary condition, which is naturally chosen to be

$$u(\tau = \infty, x) = 1/x, \quad (3.27)$$

corresponding to the relaxation of the distribution function to the final Maxwellian. Then it can be shown that (3.25) and (3.27) together rule out all similarity solutions of (3.1) except (3.20).

In view of the above conclusion, classes of similarity solutions which are not of the Krook–Wu type may have a physical meaning only if the condition of constant number density is relaxed. Then, of course, the Boltzmann equation must be modified by the addition of a source term which supplies (or subtracts) particles at an appropriate rate. Thus we must solve the equation

$$\begin{aligned} \frac{\partial f}{\partial \tau}(\tau, v) = & -f(\tau, v) \int d\mathbf{w} f(\tau, w) + \frac{1}{4\pi} \int d\mathbf{w} \int_0^\pi d\chi \sin\chi \\ & \times \int_0^{2\pi} d\epsilon f(\tau, v') f(\tau, w') + S(\tau, v), \end{aligned} \quad (3.28)$$

where $S(\tau, v)$ is an (as yet) unspecified function of time and of the speed of the particles. On taking moments, we find

$$\begin{aligned} \frac{d}{d\tau} M_n(\tau) = & -M_0(\tau) M_n(\tau) + \frac{1}{n+1} \sum_{m=0}^n M_m(\tau) M_{n-m}(\tau) \\ & + Q_n(\tau), \end{aligned} \quad (3.29)$$

where

$$Q_n(\tau) = \frac{\sqrt{\pi}}{2(2\beta^2)^n \Gamma(n + \frac{3}{2})} \int dv v^{2n} S(\tau, v). \quad (3.30)$$

Furthermore, let

$$Q_n(\tau) = -M_n(\tau)[1 - M_0(\tau)] + R_n(\tau), \quad (3.31)$$

which is equivalent to saying that $S(\tau, v)$ consists of a particular kind of sink and an arbitrary source. Then we can rewrite (3.29) as follows:

$$\frac{d}{d\tau} M_n(\tau) + M_n(\tau) = \frac{1}{n+1} \sum_{m=0}^n M_m(\tau) M_{n-m}(\tau) + R_n(\tau), \quad (3.32)$$

and, with the procedure outlined before, transform this equation into a second order p.d.e., viz.

$$u_{x\tau} + u_x + u^2 - \psi = 0, \quad (3.33)$$

where $\psi = \psi(\tau, x)$ results from the source term R . On searching for similarity solutions of (3.33), one finds now that among the set of determining equations there is a compatibility condition which ψ must satisfy, namely

$$(\gamma x + \delta) \frac{\partial \psi}{\partial x} + [\beta - \alpha \exp(\tau)] \frac{\partial \psi}{\partial \tau} = -2[\gamma - \alpha \exp(\tau)] \psi, \quad (3.34)$$

where α, β, γ , and δ are arbitrary constants. And since this is a first order linear p.d.e. it is equivalent to

$$\frac{dx}{\gamma x + \delta} = \frac{d\tau}{\beta - \alpha \exp(\tau)} = \frac{d\psi}{-2[\gamma - \alpha \exp(\tau)] \psi}, \quad (3.35)$$

from which ψ can be determined.

As an example, let $\delta = \beta = \alpha = 0$ and $\gamma = 1$. Then one finds $\psi(\tau, x) = \phi(\tau)/x^2$, and the simplest similarity solution of (3.33) is given by

$$u(\tau, x) = x^{-1} G(\tau), \quad (3.36)$$

which is of the same class as (3.21). The arbitrary function of time $\phi(\tau)$ must be prescribed. For instance, we could imagine our gas to be isolated and in equilibrium at the initial time $\tau=0$. Then a sink and a source that behave in the manner described above are switched on, and the source corresponding to $\phi(\tau)$ has a constant rate k , say. In this case

$$\phi(\tau) = kh(\tau), \quad (3.37)$$

where $h(\tau)$ is the unit step function, and the distribution function is given by

$$f(\theta, v) = \frac{1}{2} \left[1 + \left(\frac{\theta - 2}{\theta} \right) \sqrt{4k + 1} \right] \frac{\exp(-v^2/2\beta^2)}{(2\pi\beta^2)^{3/2}}, \quad (3.38)$$

where the time variable is defined as

$$\theta = 1 + c \exp(-\sqrt{4k + 1} \tau), \quad (3.39)$$

and c is a constant. Finally, since $f(\theta, v) \geq 0$ for physical reasons, we must have $-\frac{1}{4} \leq k \leq 0$, which means that the term (3.37) is a sink as well.

The solution (3.38) helps us to give meaning to the similarity solutions which are not of the Krook–Wu type. Indeed, suppose that $k=0$, i.e., $\psi=0$ in (3.33). Then the p.d.e. is formally the same as Eq. (3.1) and the solution (3.24) would correspond to the distribution function

$$f(\tau, v) = \frac{1}{\gamma} (1 + C \exp(\tau))^{-1} \frac{\exp(-v^2/2\beta^2)}{(2\pi\beta^2)^{3/2}}. \quad (3.40)$$

This solution violates the boundary condition for relaxation to equilibrium, but is consistent with (3.38), as can be seen from the latter by setting $k=0$ and redefining the constants appropriately. In other words, the classes of similarity solutions which are not of the Krook–Wu type can be regarded as exact solutions of the spatially homogeneous Boltzmann equation in the presence of particular kinds of sinks.

It should be noted that the introduction of this special kind of sinks need not be taken literally as representing some physically realistic situation. Rather it should be thought of as a conceptual device which gives meaning to some classes of exact solutions of the Boltzmann equation for the homogeneous, isotropic and pseudo-Maxwellian gas. Their possible relevance to more realistic situations will be discussed in the next section.

IV. SOLUTIONS OF THE NIKOL'SKII TYPE

Most interesting problems of kinetic theory and rarefied gas dynamics concern systems which are inhomogeneous in space, i.e. in which the system can be described by a distribution function $f(t, \mathbf{r}, \mathbf{v})$ depending on the space variable as well, and obeying the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f = \iiint (f' f'_1 - f f_1) g b d\epsilon d\mathbf{v}_1, \quad (4.1)$$

in the usual notation.²

More than a decade ago Nikol'skii⁵ noticed that if one looks for a solution of the Boltzmann equation of the form

$$f(t, \mathbf{r}, \mathbf{v}) = F[\phi(t), \gamma]; \quad \gamma \equiv t(\mathbf{v} - \mathbf{r}/t), \quad (4.2)$$

and if the interaction force is repulsive and of inverse power form, $\kappa r^{-\nu}$, then for $\nu > 2$ Eq. (4.1) becomes

$$\phi'(t) \frac{\partial F}{\partial \phi} = |t|^{4[(2-\nu)/(\nu-1)]} \iiint [F(\phi, \gamma') F(\phi, \gamma_1) - F(\phi, \gamma) F(\phi, \gamma_1)] \times |\gamma_1 - \gamma| b db d\epsilon d\gamma_1. \quad (4.3)$$

It then follows⁵ that we must have

$$\phi'(t) = |t|^{4[(2-\nu)/(\nu-1)]} \quad (4.4)$$

and

$$\frac{\partial F}{\partial \phi} = \iiint (F' F_1' - F F_1) |\gamma - \gamma_1| b db d\epsilon d\gamma_1. \quad (4.5)$$

Thus the transformation (4.2) gives a class of solutions to the complete Boltzmann equation (4.1), in which a spatially homogeneous solution of (4.5) is associated with the distribution function at each point. Consequently one can generate exact solutions for the spatially inhomogeneous problem from exact solutions of the homogeneous one.

Even without the knowledge of any exact solution of (4.5), Nikol'skii was able to discuss some properties of the distribution function (4.2). For simplicity we shall assume that $\nu = 5$, which corresponds to a model potential consistent with the cross section (1.1). Moreover we shall concentrate on those motions of the gas which occur for $t > 0$, and shall understand that the independent variables $t, \mathbf{r}, \mathbf{v}$ are expressed in dimensionless form. Then integration of (4.4) gives

$$\phi(t) = \alpha - 1/2t^2 \quad (t > 0) \quad (4.6)$$

and so the distribution function is

$$f(t, \mathbf{r}, \mathbf{v}) = F(\alpha - 1/2t^2, \gamma), \quad (4.7)$$

where the initial value of the dimensionless time variable can be taken as $t = 1$, without loss of generality.

Suppose now that one assigns the initial distribution $F(\alpha - \frac{1}{2}, \gamma)$. Obviously it describes a nonequilibrium and homogenous state of the system. According to the H theorem such a state, when left to itself, would evolve to the Maxwellian equilibrium when $\phi \rightarrow \infty$. But as (4.6) shows, the quantity $\phi(t) \rightarrow \alpha$ when $t \rightarrow \infty$. Hence the solution (4.7) of the Boltzmann equation cannot describe relaxation to equilibrium. In fact Nikol'skii shows that it corresponds to an expansion of the gas in infinite three-dimensional space. He also shows that a similar conclusion holds for arbitrary $\nu > \frac{2}{3}$, including the case $\nu \rightarrow \infty$, which corresponds to a hard-sphere potential.

In order to see more clearly what kind of motion of the gas the solutions of the Nikol'skii type do represent, it is convenient to consider the behavior of the fluid dynamic variables. Once the distribution function is known, we have for the number density

$$n \equiv \int d\mathbf{v} f(t, \mathbf{r}, \mathbf{v}) = (1/t^3) \int d\gamma F(\phi, \gamma), \quad (4.8)$$

which is seen to be independent of the space variable \mathbf{r} . This behavior is just a reflection of the fact that the Nikol'skii solutions refer to cases in which the distribution function is constrained to be the same at all points. The average flow velocity, on the other hand, does depend on the space coordinates, since we have

$$n\mathbf{u}(t, \mathbf{r}) \equiv \int d\mathbf{v} \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) = (1/t^3) \int d\gamma \left(\frac{\mathbf{r} - \gamma}{t} \right) F(\phi, \gamma), \quad (4.9)$$

and therefore, using (4.8),

$$\mathbf{u}(t, \mathbf{r}) = \frac{\mathbf{r}}{t} - \frac{1}{n} \int d\gamma \frac{\gamma}{t^2} F(\phi, \gamma). \quad (4.10)$$

Thus the gas velocity consists of two parts. The first depends on the space coordinates and is kinematical in nature. It does not depend on any dynamical quantity and its physical origin comes from the presence at \mathbf{r} of those particles which took exactly the time t to get there. The second part, instead, is dynamical in nature and does not depend on the space coordinates, again reflecting the peculiar characteristics of the Nikol'skii solutions.

We note, incidentally, that the existence of a kinematical part in the flow velocity also occurs in the case in which one considers the collisionless expansion of a gas into vacuum.⁶ It is easy to show that in that case the distribution function has the form

$$f_{\text{free}}(t, \mathbf{r}, \mathbf{v}) = G(\mathbf{r} - \mathbf{v}t, \mathbf{v}), \quad (4.11)$$

which gives for the gas velocity

$$\mathbf{u}(t, \mathbf{r}) = \frac{\mathbf{r}}{t} - \frac{1}{n} \int d\gamma' \frac{\gamma'}{t^2} G\left(\gamma', \frac{\mathbf{r} - \gamma'}{t}\right), \quad (4.12)$$

showing that the dynamical part depends on the space coordinates as well. It is interesting to observe that in the free expansion case there is a kind of "diffusion", despite the absence of collisions or walls, due exclusively to the kinematics of the flow.⁶ For the Nikol'skii solutions, instead, no such process exists (despite the fact that the effect of collisions can be taken into account exactly), since there can be no gradients in the density for these solutions.

In discussing the above solutions of Eq. (4.1) no assumption has been made as to the isotropy of the system. Now, however, we specialize further to the case in which the functional F in (4.2) is a function of $\gamma = |\gamma|$. Moreover, if the interaction law is again assumed to be pseudo-Maxwellian, then the collision integral in Eq. (4.5) can be split into two separate terms and the equation reduced to the form (2.1), that is to the starting point of the Krook-Wu method. Hence the calculations of the previous section can be repeated and the results become relevant for the search of solutions of the Nikol'skii type. We shall not go here into a discussion of any specific problem. It should be noticed, however, that for the isotropic case and spherical symmetry the flow velocity (4.12) becomes

$$\mathbf{u}(t, \mathbf{r}) = \mathbf{r}/t, \quad (4.13)$$

i. e., a particular case of $\mathbf{u} = \mathbf{r}f(t)$, where $f(t)$ is an arbitrary function. Similarity motions of this type include problems such as the propagation of a detonation wave in a medium with variable density, the problem of an intense point explosion for constant or variable initial density, and others. They have been studied in the past by Sedov⁷ from the standpoint of continuum mechanics.

V. SUMMARY AND DISCUSSION

In this paper we have studied the problem of finding classes of exact solutions of the nonlinear Boltzmann equation, assuming that the interaction law is pseudo-Maxwellian. The work was motivated by the recent paper of Krook and Wu,¹ in which they reported their discovery of a similarity solution of the velocity relaxation problem. Because of the importance of the work of Krook and Wu and the paucity of details of their paper, we thought it useful to give a derivation of their results based on well established group-theoretic techniques.

We have shown that, thanks to Carleman's theorem of existence and uniqueness, the Krook-Wu result is *the* solution of the nonlinear Boltzmann equation for the case in which the number density is constrained to being a constant at all times. Moreover, on relaxing the assumption that the system be isolated and introducing sinks and sources, we have shown that other classes of exact solutions of the Boltzmann equation do exist. These are interesting not only as mathematical curiosities, but also insofar as they are relevant to the method of Nikol'skii⁵ for generating a class of exact solutions of the spatially inhomogeneous Boltzmann equation from the knowledge of exact solutions of the homogeneous case.

The work of Nikol'skii went unnoticed, except for a mention by Kogan² concerning the case of hard-sphere

potential. The main reason for this neglect is probably due to the fact that, in the absence of exact solutions of the homogeneous problem, the analysis of Nikol'skii could not be carried further. Thanks to the work of Krook and Wu, however, we are now in a position to pursue such an analysis, as we have tried to show in this paper. Thus it seems reasonable to expect that in the near future some interesting problems of gas dynamics—of the type considered by Sedov,⁷ for example—will be successfully studied from the point of view of the Boltzmann equation and with the help of exact analytical tools.

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No-interaction theorem of Currie, Jordan, and Sudarshan. Expansions in c^{-1}

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By means of an expansion in c^{-1} (c being the velocity of light) it is shown that the no-interaction theorem of Currie, Jordan, and Sudarshan is valid only when terms of order of at least c^{-6} are included. To confirm this result, we derive the most general family of approximate Lagrangians up to order c^{-4} , whose limit is Newtonian.

1. INTRODUCTION

In predictive relativistic mechanics (PRM), the evolution of an isolated system of N structureless point particles is given^{1,2} by a system of second order ordinary differential equations of the following type:

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

$$\left(\begin{array}{l} i, j, k = 1, 2, 3 \\ a, b, c = 1, 2, \dots, N \end{array} \right),$$

where t is the time and $(x_a^i) \in \mathbb{R}^{3N}$ are the Cartesian coordinates of particle a in a Galilean frame of reference. The functions $\mu_a^i(t; x_b^j, v_c^k)$ which characterize the dynamics of the system or, in other words, the interaction of the particles should make the system (1.1) invariant under the connected component of the Poincaré group, which implies the following properties:

(a) Time does not appear explicitly in μ_a^i , that is,

$$\frac{\partial \mu_a^i}{\partial t} = 0; \quad \text{so} \quad \frac{d\mu_a^i}{dt} = \mu_a^i(x_b^j, v_c^k). \quad (1.2)$$

(b) The following vector fields on the fiber bundle $T(\mathbb{R}^{3N})$,³

$$\mathbf{H} \equiv v_a^i \frac{\partial}{\partial x_a^i} + \mu_a^i(x_b^j, v_c^k) \frac{\partial}{\partial v_a^i}, \quad (1.3a)$$

$$\mathbf{P}_j \equiv \epsilon_a \frac{\partial}{\partial x_a^j}, \quad (1.3b)$$

$$\mathbf{J}_j \equiv \eta_j^i x_a^k \frac{\partial}{\partial x_a^i} + \eta_j^i x_a^k v_a^i \frac{\partial}{\partial v_a^k}, \quad (1.3c)$$

$$\mathbf{K}_j \equiv -\frac{1}{c^2} x_{aj} v_a^i \frac{\partial}{\partial x_a^i} + \left(\epsilon_a \delta_j^i - \frac{1}{c^2} v_{aj} v_a^i - \frac{1}{c^2} x_{aj} \mu_a^i \right) \frac{\partial}{\partial v_a^i}, \quad (1.3d)$$

verify the commutation relations characteristic of the Poincaré Lie algebra, that is,

$$[\mathbf{P}_i, \mathbf{P}_j] = 0, \quad [\mathbf{J}_i, \mathbf{P}_j] = \eta_{ij}^l \mathbf{P}_l, \quad [\mathbf{J}_i, \mathbf{J}_j] = \eta_{ij}^l \mathbf{J}_l, \quad (1.4a)$$

$$[\mathbf{P}_i, \mathbf{H}] = 0, \quad [\mathbf{J}_i, \mathbf{H}] = 0, \quad [\mathbf{K}_i, \mathbf{H}] = \mathbf{P}_i, \quad (1.4b)$$

$$[\mathbf{K}_i, \mathbf{P}_j] = \frac{1}{c^2} \delta_{ij} \mathbf{H}, \quad [\mathbf{K}_i, \mathbf{J}_j] = \eta_{ij}^l \mathbf{K}_l, \quad (1.4c)$$

$$[\mathbf{K}_i, \mathbf{K}_j] = -\frac{1}{c^2} \eta_{ij}^l \mathbf{J}_l$$

where $[\ , \]$ is the Lie bracket of two vector fields.

It should be pointed out that the relations (1.4a) do

not impose any restriction on the dynamical system (1.1), because they contain only the generators of the Euclidean group, which do not depend on the functions $\mu_a^i(x_b^j, v_c^k)$ as can be seen in (1.3b) and (1.3c). However, the relations (1.4b) and (1.4c) are equivalent to the following conditions on the functions μ_a^i :

$$\mathcal{L}(\mathbf{P}_j) \mu_a^i = 0, \quad (1.5a)$$

$$\mathcal{L}(\mathbf{J}_j) \mu_a^i = \eta_j^i k \mu_a^k, \quad (1.5b)$$

$$\mathcal{L}(\mathbf{K}_j) \mu_a^i + \frac{1}{c^2} x_{aj} \mathcal{L}(\mathbf{H}) \mu_a^i = -\frac{1}{c^2} (2v_{aj} \mu_a^i + v_a^i \mu_{aj}), \quad (1.5c)$$

where $\mathcal{L}(\)$ is the Lie-derivative operator. These equations were obtained by Currie¹ and Hill⁴ as necessary conditions for the invariance of the dynamical system (1.1) under the Poincaré group; later Bel⁵ has shown that they are also sufficient conditions. The interpretation of Eqs. (1.5) is as follows:

(i) Equations (1.5a) express the invariance of the functions μ_a^i under the space translation group, that is, the functions μ_a^i actually depend on the relative positions of the particles.

(ii) Equations (1.5b) state that the μ_a^i behave as vectors under the rotation group, that is, they are vector functions of vector variables with respect to that group.

(iii) Equations (1.5c) are not easily interpreted. We will only point out that they are related to the pure Lorentz transformations (which are not a group) and to the one-parameter group of time evolution generated by \mathbf{H} . Taking into account the structure of \mathbf{H} and \mathbf{K}_j given by (1.3a) and (1.3d), it can be seen that Eqs. (1.5c) constitute a nonlinear system of partial differential equations.

Hereinafter, we will call the dynamical systems (1.1) satisfying Eqs. (1.2) and (1.4), or equivalently (1.5), Poincaré invariant predictive systems (PIPS).

One of the fundamental problems concerning the PIPS theory is to find out if such systems admit a Lagrangian (or Hamiltonian) formulation compatible with their invariance under the Poincaré group. Should the answer be affirmative, then it would be possible to define unambiguously the usual notions of energy, linear momentum, angular momentum, and center of mass, identifying them, respectively, with the generat-

ing functions of the infinitesimal canonical transformations related to time evolution, space translations, rotations and pure Lorentz transformations (in the last case except for a factor which is the total energy of the system). Unfortunately, as is well known, Currie, Jordan, and Sudarshan⁶ have shown that the usual definition of Lagrangian dynamical system leads to a no-interaction theorem, that is, the only PIPS which admit a Lagrangian formulation compatible with their invariance are the free particle systems ($\mu_a^i = 0$). However, it is also known that if one restricts himself to second order in a formal expansion in powers of c^{-1} (c being the velocity of light), he is then able to find PIPS which admit a Lagrangian formulation compatible with their invariance: Good examples are the dynamics derived from the Lagrangians of Darwin,⁷ Einstein, Infeld, and Hoffmann,⁸ Bopp,⁹ Bagge,¹⁰ etc. This fact has allowed the conjecture that, from the point of view of an expansion in $1/c$, the no-interaction theorem of Currie, Jordan and Sudarshan begins to be decisive at the *fourth* order, it then being impossible to find out about approximate Lagrangians at the fourth and higher orders.¹¹

The main purpose of this paper is to show that the mentioned conjecture is wrong and that it is actually the sixth order which gives a classical (nonrelativistic) limit of free particles. To strengthen this result, we get, by using a simple procedure, the most general family of approximate Lagrangians up to and including the fourth order, having all the desired properties. Moreover, the introduction of restrictions imposed to order c^{-4} eliminates the possibility that the known Lagrangians up to order c^{-2} are contained in the approximated Lagrangian up to order c^{-4} .

In Secs. 2 and 3 we give some results (some of them already known and some other new) which are derived from the notion of compatible Lagrangian formulation of a PIPS. These results ease the work in the following sections.

2. LAGRANGIAN FORMULATION COMPATIBLE WITH THE ARISTOTLE GROUP

(A) Let us first consider a dynamical system of type (1.1) invariant only under time translations, i. e., such that (1.2) is verified. Usually, the dynamical system (1.1) is said to admit a Lagrangian formulation compatible with (1.2) if a function $L(x_b^j, v_c^k)$ (without explicit dependence on time) exists, such that

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

As is well known, this definition is equivalent to the existence of a symplectic form σ on $T(\mathbb{R}^{3N})$, with the following structure:

$$\sigma = dx_a^i \wedge dp_i^a, \quad p_i^a = p_i^a(x_b^j, v_c^k) \quad (2.2)$$

and invariant under the one-parameter group of time evolution generated by \mathbf{H} , that is,

$$\mathcal{L}(\mathbf{H})\sigma = 0. \quad (2.3)$$

We will carry out the proof of this equivalence for its later usage.

Condition (2.3), together with (2.2), give the equations

$$\frac{\partial}{\partial x_b^j} \mathcal{L}(\mathbf{H}) p_i^a - \frac{\partial}{\partial x_a^i} \mathcal{L}(\mathbf{H}) p_j^b = 0, \quad (2.4a)$$

$$\frac{\partial p_i^a}{\partial x_b^j} - \frac{\partial p_j^b}{\partial x_a^i} = 0, \quad (2.4b)$$

$$\frac{\partial}{\partial v_b^j} \mathcal{L}(\mathbf{H}) p_i^a - \frac{\partial p_j^b}{\partial x_a^i} = 0. \quad (2.4c)$$

From (2.4a) and (2.4b) it can be deduced that there exist functions $A(x_b^j, v_c^k)$ and $B(x_b^j, v_c^k)$, defined except for the transformation,

$$A \rightarrow A + \Phi(v_c^k), \quad B \rightarrow B + \Psi(x_b^j), \quad (2.5)$$

in such a way that

$$\mathcal{L}(\mathbf{H}) p_i^a = \frac{\partial A}{\partial x_a^i}, \quad p_i^a = \frac{\partial B}{\partial v_a^i}. \quad (2.6)$$

Using this result and (2.4c), we have

$$\frac{\partial^2(A - B)}{\partial x_a^i \partial v_b^j} = 0 \Rightarrow A - B = \hat{\Phi}(v_c^k) + \hat{\Psi}(x_b^j). \quad (2.7)$$

Realizing the arbitrariness (2.5), it is possible to choose $A = B \equiv L(x_b^j, v_c^k)$; after (2.6) and the fact that σ is of maximum rank, we get the relations (2.1). Conversely, let us suppose the existence of a Lagrangian $L(x_b^j, v_c^k)$ verifying (2.1); it is evident that the exterior differential 2-form defined by

$$\sigma \equiv dx_a^i \wedge d \frac{\partial L}{\partial v_a^i} \quad (2.8)$$

is symplectic and has the structure (2.2); moreover, after taking into consideration (2.1), we have

$$\mathcal{L}(\mathbf{H})\sigma = dv_a^i \wedge d \frac{\partial L}{\partial v_a^i} + dx_a^i \wedge d \frac{\partial L}{\partial x_a^i} \equiv 0. \quad (2.9)$$

QED

It is interesting to point out the fact that given a symplectic form σ of type (2.2), the functions $p_i^a(x_b^j, v_c^k)$ are defined except for the transformation

$$p_i^a \rightarrow p_i^a + \frac{\partial}{\partial x_a^i} S(x_b^j), \quad (2.10)$$

and then the Lagrangian is defined except for the transformation

$$L \rightarrow L + \mathcal{L}(\mathbf{D}) S(x_b^j), \quad \mathbf{D} \equiv v_a^i \frac{\partial}{\partial x_a^i}. \quad (2.11)$$

(B) Let us now suppose that the dynamical system (1.1) is invariant under the Aristotle group (Euclidean group and time translations), i. e., such that (1.2) as well as the first two relations of (1.4b) [or either (1.5a) and (1.5b)] are satisfied. In this situation we will say that the dynamical system admits a Lagrangian formulation compatible with its invariance under the Aristotle group, if there exists a symplectic form of type (2.2), verifying (2.3) and

$$\mathcal{L}(\mathbf{P}_j)\sigma = 0, \quad \mathcal{L}(\mathbf{J}_j)\sigma = 0. \quad (2.12)$$

These relations mean that the Euclidean group acts as a canonical transformation group.

Next, we will show the following theorem¹²:

Theorem 2.1: If a symplectic form of type (2.2) verifies the conditions (2.12), then it is always possible to choose the functions $p_i^a(x_b^k, v_c^k)$ in such a way that

$$\epsilon(\mathbf{P}_j) p_i^a = 0, \quad \epsilon(\mathbf{J}_j) p_i^a = \eta_{ji}^k p_k^a, \quad (2.13)$$

that is, such that they are invariant under space translations and they behave as vectors under the rotation group. Once this choice has been made, the arbitrariness (2.10) still persists, but now with the condition

$$\epsilon(\mathbf{P}_j) S(x_b^k) = 0, \quad \epsilon(\mathbf{J}_j) S(x_b^k) = 0. \quad (2.14)$$

Proof: The conditions (2.12), taking into account (2.2), lead straightforwardly to the following equations:

$$\frac{\partial}{\partial x_b^k} \epsilon(\mathbf{P}_j) p_i^a - \frac{\partial}{\partial x_a^i} \epsilon(\mathbf{P}_j) p_k^b = 0, \quad (2.15)$$

$$\frac{\partial}{\partial v_b^k} \epsilon(\mathbf{P}_j) p_i^a = 0,$$

$$\frac{\partial}{\partial x_b^k} [\epsilon(\mathbf{J}_j) p_i^a - \eta_{ji}^l p_l^a] - \frac{\partial}{\partial x_a^i} [\epsilon(\mathbf{J}_j) p_k^b - \eta_{jk}^l p_l^b] = 0, \quad (2.16)$$

$$\frac{\partial}{\partial v_b^k} [\epsilon(\mathbf{J}_j) p_i^a - \eta_{ji}^l p_l^a] = 0,$$

from which we deduce that there functions $F_j(x_b^k)$ and $Q_j(x_b^k)$ exist, defined except for additive constants, such that

$$\epsilon(\mathbf{P}_j) p_i^a = \frac{\partial}{\partial x_a^i} F_j(x_b^k), \quad (2.17a)$$

$$\epsilon(\mathbf{J}_j) p_i^a - \eta_{ji}^l p_l^a = \frac{\partial}{\partial x_a^i} Q_j(x_b^k). \quad (2.17b)$$

Taking into account (1.4a), the integrability conditions of (2.17) trivially give the following relations:

$$\epsilon(\mathbf{P}_j) F_i - \epsilon(\mathbf{P}_i) F_j = a_{ji} \quad (\text{const}), \quad (2.18a)$$

$$\epsilon(\mathbf{J}_j) Q_i - \epsilon(\mathbf{J}_i) Q_j - \eta_{ji}^l Q_l = b_{ji} \quad (\text{const}), \quad (2.18b)$$

$$\epsilon(\mathbf{J}_j) F_i - \epsilon(\mathbf{P}_i) Q_j - \eta_{ji}^l F_l = c_{ji} \quad (\text{const}); \quad (2.18c)$$

now, since the constants b_{ji} must be skew-symmetric, it is always possible to redefine the functions $Q_i(x_b^k)$ such that $Q_i \rightarrow Q_i - b_i$, with $b_i \equiv \frac{1}{2} \eta^{ji} b_{ji}$. Then Eq. (2.18b) reads

$$\epsilon(\mathbf{J}_j) Q_i - \epsilon(\mathbf{J}_i) Q_j = \eta_{ji}^l Q_l. \quad (2.18b')$$

On the other hand, by taking into account (1.4a), the general solutions of (2.18a) and (2.18b') can be written as follows:

$$F_j(x_b^k) = \epsilon(\mathbf{P}_j) F(x_b^k) + (1/2N) a_{ij} \epsilon^a x_a^i, \quad (2.19)$$

$$Q_j(x_b^k) = \epsilon(\mathbf{J}_j) Q(x_b^k),$$

where N is the number of particles and the functions $F(x_b^k)$ and $Q(x_b^k)$ are defined except for the transformation:

$$F \rightarrow F + R(x_b^k), \quad \epsilon(\mathbf{P}_j) R = 0, \quad (2.20)$$

$$Q \rightarrow Q + T(x_b^k), \quad \epsilon(\mathbf{J}_j) T = 0.$$

Upon introducing (2.19) in (2.18c) and taking into account the second relation in (1.4a), one obtains

$$\epsilon(\mathbf{P}_i) \epsilon(\mathbf{J}_j) (F - Q) = c_{ji} - (1/2N) (a_{ii} \eta_j^i - a_{ik} \eta_j^i) \epsilon^a x_a^k \quad (2.21)$$

whose integrability conditions give, after a simple calculation,

$$a_{ji} = 0, \quad (2.22a)$$

$$c_{ji} + c_{ij} = 0. \quad (2.22b)$$

The relation (2.22b) states that constants c_{ji} must be skew-symmetric, which implies that it is always possible to redefine the functions $F_i(x_b^k)$ such that $F_i \rightarrow F_i - c_i$, with $c_i \equiv \frac{1}{2} \eta_i^{ji} c_{ji}$. Then the second member of (2.18c) vanishes, so that one can always assume that those constant are zero. Then, we conclude that Eq. (2.21) reduces to the following one:

$$\epsilon(\mathbf{P}_i) \epsilon(\mathbf{J}_j) (F - Q) = 0, \quad (2.21')$$

whose general solution can be written as follows:

$$F - Q = \hat{R}(x_b^k) + \hat{T}(x_b^k), \quad \epsilon(\mathbf{P}_j) \hat{R} = 0, \quad \epsilon(\mathbf{J}_j) \hat{T} = 0. \quad (2.23)$$

Thus, taking into account the arbitrariness (2.20), it is always possible to choose $F = Q \equiv -S(x_b^k)$, and then from (2.19) and (2.22a), Eqs. (2.17) read as follows:

$$\epsilon(\mathbf{P}_j) \left[p_i^a + \frac{\partial S}{\partial x_a^i} \right] = 0, \quad (2.24)$$

$$\epsilon(\mathbf{J}_j) \left[p_i^a + \frac{\partial S}{\partial x_a^i} \right] = \eta_{ji}^l \left[p_l^a + \frac{\partial S}{\partial x_a^l} \right],$$

which demonstrate the first part of the theorem [considering the arbitrariness (2.10) in the definition of the functions $p_i^a(x_b^k, v_c^k)$]. The proof that this arbitrariness remains [but with condition (2.14)] is easily obtained.

QED

We are now able to prove the main result of this section, which is given in the following theorem:

Theorem 2.2: A necessary and sufficient condition for the dynamical system (1.1) to be invariant under the Aristotle group and to admit a Lagrangian formulation compatible with its invariance is the existence of a Lagrangian $L(x_b^k, v_c^k)$, such that it verifies (2.1) and

$$\epsilon(\mathbf{P}_j) L = 0, \quad \epsilon(\mathbf{J}_j) L = 0, \quad (2.25)$$

that is, invariant under space translation and rotations. For a given Lagrangian formulation, the Lagrangian is defined except for the transformation

$$L \rightarrow L + \epsilon(\mathbf{D}) S(x_b^k), \quad \epsilon(\mathbf{P}_j) S = \epsilon(\mathbf{J}_j) S = 0. \quad (2.26)$$

Proof: We will show first that the condition is necessary. From subsection (A) of this section, we see that $L(x_b^k, v_c^k)$ verifying (2.1) exists. Thus, from Theorem 2.1, we have

$$\epsilon(\mathbf{H}) p_i^a = \frac{\partial L}{\partial x_a^i}, \quad (2.27a)$$

$$\epsilon(\mathbf{P}_j) p_i^a = 0, \quad (2.27b)$$

$$\epsilon(\mathbf{J}_j) p_i^a = \eta_{ji}^l p_l^a, \quad (2.27c)$$

with

$$p_i^a \equiv \frac{\partial L}{\partial v_a^i}. \quad (2.28)$$

Taking into account the invariance of the dynamical

system under the Euclidean group, that is, the first two relations of (1.4b), the integrability conditions of (2.27) read as follows:

$$\frac{\partial}{\partial x_a^i} \mathcal{L}(\mathbf{P}_j) L = 0, \quad \frac{\partial}{\partial x_a^i} \mathcal{L}(\mathbf{J}_j) L = 0. \quad (2.29)$$

On the other hand, using (2.28), Eqs. (2.27b) and (2.27c) directly give the following relations:

$$\frac{\partial}{\partial v_a^i} \mathcal{L}(\mathbf{P}_j) L = 0, \quad \frac{\partial}{\partial v_a^i} \mathcal{L}(\mathbf{J}_j) L = 0. \quad (2.30)$$

From (2.29) and (2.30), one obtains

$$\mathcal{L}(\mathbf{P}_j) L = a_j \text{ (const)}, \quad \mathcal{L}(\mathbf{J}_j) L = b_j \text{ (const)}, \quad (2.31)$$

whose integrability conditions require that $a_j = b_j = 0$.

Next, we will show the sufficiency: We need only show that the dynamical system is invariant under the Aristotle group, since the symplectic form defined by (2.8) verifies (2.3) and (2.12) as a consequence of the results of subsection (A) and of (2.25). First, one has the following identities:

$$\begin{aligned} \mathcal{L}(\mathbf{P}_j, \mathbf{H}) x_a^i &= 0, \\ \mathcal{L}(\mathbf{J}_j, \mathbf{H}) x_a^i &= \eta_j^i v_a^i - \eta_j^i v_a^i = 0, \end{aligned} \quad (2.32)$$

and, on the other hand, taking into account (2.1) and (2.25), one easily obtains

$$\mathcal{L}(\mathbf{P}_j, \mathbf{H}) p_i^a = 0, \quad \mathcal{L}(\mathbf{J}_j, \mathbf{H}) p_i^a = 0; \quad (2.33)$$

now, as a consequence of the second condition of (2.1), $\{x_a^i, p_j^b\}$ constitutes a coordinate system (not adapted) of $T(\mathbb{R}^{3N})$, and therefore, (2.32) and (2.33) imply

$$[\mathbf{P}_j, \mathbf{H}] = 0, \quad [\mathbf{J}_j, \mathbf{H}] = 0, \quad (2.34)$$

that is, the dynamical system is invariant under the Euclidean group. The invariance under time translations turns out to be trivial. Finally, the arbitrariness (2.26) is an immediate consequence of Theorem 2.1.

QED

3. LAGRANGIAN FORMULATION COMPATIBLE WITH THE POINCARÉ GROUP

(A) In this section we will suppose that the dynamical system (1.1) is a PIPS, that is, such that it verifies (1.2) and (1.4), or (1.5) which is the same. Then we will say that the dynamical system admits a Lagrangian formulation compatible with its invariance if there exists a symplectic form σ of type (2.2) such that it verifies relations (2.3), (2.12), and also the following one:

$$\mathcal{L}(\mathbf{K}_j) \sigma = 0, \quad (3.1)$$

that is to say, the whole Poincaré group acts as a canonical transformation group.

Essentially, the new conditions appearing in this section are (1.5c) and (3.1), our goal being to exploit them as much as possible. Taking into account (1.3d) and (2.2), Eq. (3.1) gives the following equations:

$$\frac{\partial}{\partial x_b^i} \mathcal{L}(\mathbf{K}_j) p_i^a - \frac{\partial}{\partial x_a^i} \mathcal{L}(\mathbf{K}_j) p_i^b - \delta_{ji} v^{ak} \frac{\partial \tilde{p}_k^a}{\partial x_b^i} + \delta_{ji} v^{bk} \frac{\partial \tilde{p}_k^b}{\partial x_a^i} = 0, \quad (3.2a)$$

$$x_j^a \frac{\partial \tilde{p}_i^a}{\partial v_b^i} - x_j^b \frac{\partial \tilde{p}_i^b}{\partial v_a^i} = 0, \quad (3.2b)$$

$$\frac{\partial}{\partial v_b^i} \mathcal{L}(\mathbf{K}_j) p_i^a - \delta_{ji} v^{ak} \frac{\partial \tilde{p}_k^a}{\partial v_b^i} + x_j^b \frac{\partial \tilde{p}_i^b}{\partial x_a^i} = 0, \quad (3.2c)$$

where we have used the notation

$$\tilde{p}_i^a \equiv (1/c^2) p_i^a, \quad (3.3)$$

simply to avoid false information in (3.2b) concerning series expansion in powers of c^{-1} which appear below.

The results of Sec. 2 ensure the existence of a Lagrangian $L(x_b^j, v_c^k)$, defined except for the transformation (2.26), verifying (2.28) as well as (2.1) and (2.25). Then, using (2.28), Eq. (3.2b) can be written as follows:

$$(x_j^a - x_j^b) \frac{\partial^2 \tilde{L}}{\partial v_b^i \partial v_a^i} = 0, \quad \tilde{L} \equiv (1/c^2) L, \quad (3.4)$$

from which we deduce that

$$\tilde{L}(x_b^j, v_c^k) = \epsilon^a \tilde{L}_a(x_b^j, v_c^k), \quad (3.5)$$

that is to say, the "Lagrangian" \tilde{L} is the sum of N "partial Lagrangians" in such a way that each of them contains the velocity of *one* particle. Next, we prove two lemmas which will be very useful in later developments.

Lemma 3.1: The "partial Lagrangians" $\tilde{L}_a(x_b^j, v_c^k)$ are defined except for the transformation (in an evident notation):

$$\begin{aligned} \tilde{L}_a &\rightarrow \tilde{L}_a + \tilde{Q}_a(x_b^j) + v_a^k \frac{\partial}{\partial x^{ak}} S(x_b^j), \\ \epsilon^a \tilde{Q}_a &= 0, \quad \mathcal{L}(\mathbf{P}_j) \tilde{S} = \mathcal{L}(\mathbf{J}_j) \tilde{S} = 0. \end{aligned} \quad (3.6)$$

Proof: Taking into account (2.26) and (3.5), it is easy to see that the arbitrariness in the definition of \tilde{L}_a is given by (3.6); notice, however, that the function \tilde{Q}_a can also depend on v_a^i . Now, after (3.5), we have¹³

$$\tilde{p}_i^a = \frac{\partial \tilde{L}}{\partial v_a^i} = \frac{\partial \tilde{L}_a}{\partial v_a^i}; \quad (3.7)$$

thus, taking into account the arbitrariness (2.10) in the definition of p_i^a , we get

$$\tilde{p}_i^a + \frac{\partial \tilde{S}}{\partial x_a^i} = \frac{\partial \tilde{L}_a}{\partial v_a^i} + \frac{\partial \tilde{Q}_a}{\partial v_a^i} + \frac{\partial \tilde{S}}{\partial x_a^i}, \quad (3.8)$$

from which we obtain

$$\frac{\partial \tilde{Q}_a}{\partial v_a^i} = 0. \quad (3.9)$$

QED

Lemma 3.2: The "partial Lagrangian" $\tilde{L}_a(x_b^j, v_c^k)$ can always be chosen such that

$$\mathcal{L}(\mathbf{P}_j) \tilde{L}_a = 0, \quad \mathcal{L}(\mathbf{J}_j) \tilde{L}_a = 0. \quad (3.10)$$

Once this choice has been made, the arbitrariness (3.6) remains, but now with the condition

$$\mathcal{L}(\mathbf{P}_j) \tilde{Q}_a = \mathcal{L}(\mathbf{J}_j) \tilde{Q}_a = 0. \quad (3.11)$$

Proof: Taking into account (2.13) and (3.7), we easily obtain:

$$\frac{\partial}{\partial v_a^i} \mathcal{L}(\mathbf{P}_j) \tilde{L}_a = 0, \quad \frac{\partial}{\partial v_a^i} \mathcal{L}(\mathbf{J}_j) \tilde{L}_a = 0. \quad (3.12)$$

Therefore, after (2.25) and (3.5), there exist functions $\tilde{M}_j^a(x_b^k)$ and $\tilde{N}_j^a(x_b^k)$, such that

$$\underline{\epsilon}(\mathbf{P}_j) \tilde{L}^a = \tilde{M}_j^a(x_b^k), \quad \epsilon_a \tilde{M}_j^a = 0, \quad (3.13a)$$

$$\underline{\epsilon}(\mathbf{J}_j) \tilde{L}^a = \tilde{N}_j^a(x_b^k), \quad \epsilon_a \tilde{N}_j^a = 0. \quad (3.13b)$$

The integrability conditions of (3.13a) give the following equations:

$$\underline{\epsilon}(\mathbf{P}_i) \tilde{M}_j^a - \underline{\epsilon}(\mathbf{P}_j) \tilde{M}_i^a = 0, \quad (3.14)$$

$$\underline{\epsilon}(\mathbf{J}_i) \tilde{M}_j^a - \underline{\epsilon}(\mathbf{P}_j) \tilde{N}_i^a = \eta_{ij}^i \tilde{M}_i^a,$$

$$\underline{\epsilon}(\mathbf{J}_i) \tilde{N}_j^a - \underline{\epsilon}(\mathbf{J}_j) \tilde{N}_i^a = \eta_{ij}^i \tilde{N}_i^a;$$

this implies the existence of functions $\tilde{M}^a(x_b^k)$ and $\tilde{N}^a(x_b^k)$, defined except for the transformation:

$$\begin{aligned} \tilde{M}^a &\rightarrow \tilde{M}^a + \tilde{R}^a(x_b^k), \quad \underline{\epsilon}(\mathbf{P}_j) \tilde{R}^a = 0, \\ \tilde{N}^a &\rightarrow \tilde{N}^a + \tilde{T}^a(x_b^k), \quad \underline{\epsilon}(\mathbf{J}_j) \tilde{T}^a = 0, \end{aligned} \quad (3.15)$$

such that

$$\tilde{M}_j^a = \underline{\epsilon}(\mathbf{P}_j) \tilde{M}^a, \quad \tilde{N}_j^a = \underline{\epsilon}(\mathbf{J}_j) \tilde{N}^a, \quad (3.16a)$$

$$\underline{\epsilon}(\mathbf{P}_j) \underline{\epsilon}(\mathbf{J}_i) (\tilde{M}^a - \tilde{N}^a) = 0. \quad (3.16b)$$

Then, after (3.13b), it is always possible to choose $\tilde{M}^a = \tilde{N}^a = -\tilde{Q}^a(x_b^k)$ in such a way that $\epsilon^a \tilde{Q}_a = 0$. Hence, Eqs. (3.13a) can be rewritten as follows:

$$\left. \begin{aligned} \underline{\epsilon}(\mathbf{P}_j) (\tilde{L}^a + \tilde{Q}^a) &= 0 \\ \underline{\epsilon}(\mathbf{J}_j) (\tilde{L}^a + \tilde{Q}^a) &= 0 \end{aligned} \right\}, \quad \epsilon_a \tilde{Q}^a = 0 \quad (3.17)$$

It suffices now to take into account Lemma 3.1 in order to obtain the wanted result.

QED

Now we will use Eqs. (3.2a) and (3.2c). The first is equivalent to stating that functions $\Psi_j(x_b, v_c^k)$ exist, defined except for the transformation

$$\Psi_j \rightarrow \Psi_j + \Gamma_j(v_c^k), \quad (3.18)$$

such that

$$\underline{\epsilon}(\mathbf{K}_j) p_i^a - \delta_{ji} v^{ak} \tilde{p}_k^a = \frac{\partial \Psi_j}{\partial x_a^i}. \quad (3.19)$$

By introducing this result in (3.2c), and considering (3.5) and (3.7), we get

$$\frac{\partial^2}{\partial x_a^i \partial v_b^i} (x_j^c \tilde{L}_c + \Psi_j) = 0. \quad (3.20)$$

The general solution of (3.20) can be written as follows:

$$x_j^b \tilde{L}_b + \Psi_j(x_a^i, v_c^k) = \Phi_j(x_a^i) + \hat{\Gamma}(v_c^k); \quad (3.21)$$

hence, after the arbitrariness (3.18), it is always possible to assume the following structure for the functions Ψ_j :

$$\Psi_j(x_a^i, v_c^k) = -x_j^b \tilde{L}_b + \Phi_j(x_a^i). \quad (3.22)$$

Introducing now (3.22) into (3.19), we get the equation

$$\underline{\epsilon}(\mathbf{K}_j) p_i^a = \delta_{ji} v^{ak} \tilde{p}_k^a - \frac{\partial}{\partial x_a^i} (x_j^b \tilde{L}_b) + \frac{\partial \Phi_j(x_a^k)}{\partial x_a^i}. \quad (3.23)$$

Let us express the integrability conditions of (2.27a), (2.27b), and (3.23) concerning the third commutation relation of (1.4b) [which is strictly equivalent to (1.5c)]. In this way we obtain, after an easy calculation,

$$\frac{\partial}{\partial x_c^k} [\underline{\epsilon}(\mathbf{K}_j) L + \underline{\epsilon}(\mathbf{H})(x_j^b \tilde{L}_b) - \underline{\epsilon}(\mathbf{D}) \Phi_j] = 0. \quad (3.24)$$

On the other hand, using (2.28), Eq. (3.23) directly gives

$$\frac{\partial}{\partial v_c^k} [\underline{\epsilon}(\mathbf{K}_j) L + \underline{\epsilon}(\mathbf{H})(x_j^b \tilde{L}_b) - \underline{\epsilon}(\mathbf{D}) \Phi_j] = 0. \quad (3.25)$$

After (3.24) and (3.25) one obtains

$$\underline{\epsilon}(\mathbf{K}_j) L = -\underline{\epsilon}(\mathbf{H})(x_j^b \tilde{L}_b) + \underline{\epsilon}(\mathbf{D}) \Phi_j + a_j, \quad (3.26)$$

where the a_j are constants. Now, taking into account Lemma 3.2, the integrability conditions of (2.25) and (3.26), concerning the first two commutation relations of (1.4c), very easily give the following conclusions:

$$a_j = 0, \quad \Phi_j(x_c^k) = A_a x_j^a + \chi_j(x_c^k) + b_j, \quad (3.27)$$

where A^a and b^j are constants, and the functions $\chi_j(x_c^k)$ must be invariant under translations and must behave as vectors under rotations, that is,

$$\underline{\epsilon}(\mathbf{P}_i) \chi_j = 0, \quad \underline{\epsilon}(\mathbf{J}_i) \chi_j = \eta_{ij}^i \chi_i. \quad (3.28)$$

Hence, introducing (3.27) into (3.26), we get the following equation (which will be of great interest):

$$\underline{\epsilon}(\mathbf{K}_j) L = -\underline{\epsilon}(\mathbf{H})(x_j^b \tilde{L}_b) + A_b v_j^b + \underline{\epsilon}(\mathbf{D}) \chi_j. \quad (3.29)$$

Now, there only remains to use the third commutation relation of (1.4c). To do this, it is better to directly impose the corresponding integrability condition on Eq. (3.23). So one obtains, taking into account (3.27) and (3.28), the following relation (the calculation is quite tedious but easy):

$$\begin{aligned} \underline{\epsilon}(\mathbf{K}_i) \chi_j - \underline{\epsilon}(\mathbf{K}_j) \chi_i &= \underline{\epsilon}(\mathbf{K}_i)(x_j^b \tilde{L}_b) - \underline{\epsilon}(\mathbf{K}_j)(x_i^b \tilde{L}_b) \\ &\quad + (1/c^2) A_b (x_i^b v_j^b - x_j^b v_i^b). \end{aligned} \quad (3.30)$$

All these results can be summarized in the following theorem:

Theorem 3.1 (direct): If a PIPS admits a Lagrangian formulation compatible with its invariance, then a Lagrangian $L(x_b^i, v_c^k)$ exists, such that

$$\tilde{L}(x_b^i, v_c^k) = \epsilon^a \tilde{L}_a(x_b^i, v_c^k), \quad \underline{\epsilon}(\mathbf{P}_j) \tilde{L}_a = \underline{\epsilon}(\mathbf{J}_j) \tilde{L}_a = 0, \quad (3.31a)$$

$$\underline{\epsilon}(\mathbf{H}) \frac{\partial L}{\partial v_a^i} = \frac{\partial L}{\partial x_a^i}, \quad \det \left(\frac{\partial^2 L}{\partial v_a^i \partial v_b^j} \right) \neq 0, \quad (3.31b)$$

$$\underline{\epsilon}(\mathbf{P}_j) L = \underline{\epsilon}(\mathbf{J}_j) L = 0, \quad (3.31c)$$

$$\underline{\epsilon}(\mathbf{K}_j) L = -\underline{\epsilon}(\mathbf{H})(x_j^b \tilde{L}_b) + A_b v_j^b + \underline{\epsilon}(\mathbf{D}) \chi_j(x_c^k), \quad (3.31d)$$

where the A_b are constants and the functions $\chi_j(x_c^k)$ must verify the conditions (3.28) and (3.30). For a given Lagrangian formulation σ , the Lagrangian L is defined except for the transformation (2.26) and the "partial Lagrangians" \tilde{L}_a except for the transformation (3.6).

We now show the reciprocal theorem:

Theorem 3.1 (reciprocal): A sufficient condition for the dynamical system (1.1) to be a PIPS and admit a Lagrangian formulation compatible with its invariance is that a Lagrangian $L(x_b^i, v_c^k)$ verifying equations (3.31) exist.

Proof: Taking into account Theorem 2.2, we must now only prove the third commutation relation of (1.4b)

[strictly equivalent to (1.5c)], because the symplectic form defined by (2.8) verifies condition (3.1). First of all, we have the identity

$$\begin{aligned} \underline{\epsilon}([\mathbf{K}_j, \mathbf{H}] - \mathbf{P}_j) x_a^i &= \epsilon_a \delta_j^i - (1/c^2) v_{aj} v_a^i - (1/c^2) x_{aj} \mu_a^i \\ &+ (1/c^2) v_{aj} v_a^i + (1/c^2) x_{aj} \mu_a^i - \epsilon_a \delta_j^i = 0, \end{aligned} \quad (3.32)$$

and, on the other hand, taking into account (3.31), we easily get

$$\underline{\epsilon}([\mathbf{K}_j, \mathbf{H}] - \mathbf{P}_j) p_i^a = 0. \quad (3.33)$$

Since $\{x_a^i, p_j^b\}$ constitutes a coordinate system (non-adapted) of $T(\mathbb{R}^{3N})$, we get

$$[\mathbf{K}_j, \mathbf{H}] = \mathbf{P}_j. \quad (3.34)$$

QED

(B) Let us consider now a PIPS admitting a Lagrangian formulation compatible with its invariance, and let us assume that the functions $\mu_a^i(x_j^i, v_a^i)$, as well as the Lagrangian $L(x_j^i, v_a^i)$, admit a formal series expansion in powers of $1/c$ with the following structure:

$$\mu_a^i = \sum_{n=0}^{\infty} \frac{1}{c^n} \mu_a^{(n)i}, \quad L = \sum_{n=0}^{\infty} \frac{1}{c^n} L^{(n)}, \quad (3.35)$$

where the different terms $\mu_a^{(n)i}$ and $L^{(n)}$ are, of course, independent of c . In this subsection we will study of consequences of imposing Eqs. (3.31), (3.28), and (3.30) on expansions (3.35) at each order. Keeping this in mind, we will assume that constants A_b and functions $\chi_j(x_k^i)$ admit also expansions of the type:

$$A_b = \sum_{n=0}^{\infty} \frac{1}{c^n} A_b^{(n)}, \quad \chi_j = \sum_{n=0}^{\infty} \frac{1}{c^n} \chi_j^{(n)}. \quad (3.36)$$

Let us introduce, according to (1.3a) and (1.3d), the following notations:

$$\mathbf{H}^{(0)} \equiv v_a^i \frac{\partial}{\partial x_a^i} + \mu_a^{(0)i} \frac{\partial}{\partial v_a^i}, \quad \mathbf{H}^{(n)} \equiv \mu_a^{(n)i} \frac{\partial}{\partial v_a^i} \quad (n \geq 1),$$

$$\mathbf{K}_j^{(0)} \equiv \mathbf{G}_j \equiv \epsilon_a \frac{\partial}{\partial v_a^i} \quad (\text{the generators of the pure Galilean transformations}), \quad (3.37)$$

$$\mathbf{K}_j^{(2)} \equiv -x_{aj} v_a^i \frac{\partial}{\partial x_a^i} - (v_{aj} v_a^i + x_{aj} \mu_a^{(0)i}) \frac{\partial}{\partial v_a^i},$$

$$\mathbf{K}_j^{(n)} \equiv -x_{aj} \mu_a^{(n-2)i} \frac{\partial}{\partial v_a^i} \quad (n \geq 3).$$

Then Eqs. (3.31), (3.28), and (3.30) can be written at each order as follows:

Zeroth order:

$$\begin{aligned} \underline{\epsilon}(\mathbf{H}^{(0)}) \frac{\partial L^{(0)}}{\partial v_a^i} &= \frac{\partial L^{(0)}}{\partial x_a^i}, \\ \underline{\epsilon}(\mathbf{P}_j) L^{(0)} &= \underline{\epsilon}(\mathbf{J}_j) L^{(0)} = 0, \\ \underline{\epsilon}(\mathbf{G}_j) L^{(0)} &= A_b^{(0)} v_j^b + \underline{\epsilon}(\mathbf{D}) \chi_j^{(0)}, \end{aligned} \quad (3.38)$$

where the functions $\chi_j^{(0)}$ verify equations analogous to (3.28). Let us note that (3.38) are the known formulas of Galilean mechanics, so that constants $A_b^{(0)}$ can be identified with the masses of the particles.

First order: We obtain equations similar to (3.38),

except that there are two terms in the lhs of the first equation.

nth order ($n \geq 2$):

$$L^{(n-2)}(x_b^i, v_a^i) = \epsilon^a L_a^{(n-2)}(x_b^i, v_a^i), \quad \underline{\epsilon}(\mathbf{P}_j) L_a^{(n-2)} = \underline{\epsilon}(\mathbf{J}_j) L_a^{(n-2)} = 0, \quad (3.39a)$$

$$\sum_{r+s=n} \underline{\epsilon}(\mathbf{H}^{(r)}) \frac{\partial L^{(s)}}{\partial v_a^i} = \frac{\partial L^{(n)}}{\partial x_a^i}, \quad (3.39b)$$

$$\underline{\epsilon}(\mathbf{P}_j) L^{(n)} = \underline{\epsilon}(\mathbf{J}_j) L^{(n)} = 0, \quad (3.39c)$$

$$\begin{aligned} \sum_{r+s=n} \underline{\epsilon}(\mathbf{K}_j^{(r)}) L^{(s)} &= \sum_{r+s=n-2} \underline{\epsilon}(\mathbf{H}^{(r)}) (x_j^b L_b^{(s)}) \\ &+ A_b^{(n)} v_j^b + \underline{\epsilon}(\mathbf{D}) \chi_j^{(n)}, \end{aligned} \quad (3.39d)$$

where, by definition, $\mathbf{K}_j^{(1)} \equiv 0$ and functions $\chi_j^{(n)}$ verify equations analogous to (3.28) as well as the following condition coming from (3.30):

$$\begin{aligned} \underline{\epsilon}(\mathbf{K}_i^{(2)}) \chi_j^{(n-2)} - \underline{\epsilon}(\mathbf{K}_j^{(2)}) \chi_i^{(n-2)} \\ = \sum_{r+s=n-2} \{ \underline{\epsilon}(\mathbf{K}_i^{(r)}) (x_j^b L_b^{(s)}) - \underline{\epsilon}(\mathbf{K}_j^{(r)}) (x_i^b L_b^{(s)}) \} \\ + A_b^{(n-2)} (x_i^b v_j^b - x_j^b v_i^b). \end{aligned} \quad (3.40)$$

Note that conditions (3.30) and (3.31a) begin to be relevant from order $n=2$ on.

Let us now see how Eqs. (3.39d) and (3.40) can be simplified, by using the arbitrariness (2.26) and (3.6) [with (3.11)] in the definitions of L and \tilde{L}_a respectively. To do this, it is easier to handle directly the exact equations (3.30) and (3.31d), which, taking into account the mentioned arbitrariness, can also be written as follows:

$$\underline{\epsilon}(\mathbf{K}_j) L = -\underline{\epsilon}(\mathbf{H}) [x_j^b (\tilde{L}_b - A_b)] + \underline{\epsilon}(\mathbf{D}) (\chi_j - x_j^b \tilde{Q}_b), \quad (3.41)$$

$$\begin{aligned} \underline{\epsilon}(\mathbf{K}_i) (\chi_j - x_j^b \tilde{Q}_b) - \underline{\epsilon}(\mathbf{K}_j) (\chi_i - x_i^b \tilde{Q}_b) \\ = \underline{\epsilon}(\mathbf{K}_i) [x_j^b (\tilde{L}_b - A_b)] - \underline{\epsilon}(\mathbf{K}_j) [x_i^b (\tilde{L}_b - A_b)]. \end{aligned} \quad (3.42)$$

Equation (3.41) at orders $n \geq 2$ implies

$$\begin{aligned} \sum_{r+s=n} \underline{\epsilon}(\mathbf{K}_j^{(r)}) L^{(s)} = - \sum_{r+s=n-2} \underline{\epsilon}(\mathbf{H}^{(r)}) [x_j^b (L_b^{(s)} - A_b^{(s-2)})] \\ + \underline{\epsilon}(\mathbf{D}) (\chi_j^{(n)} - x_j^b Q_b^{(n-2)}). \end{aligned} \quad (3.43)$$

Furthermore, Eq. (3.42) at orders $n=2, 3$ and $n \geq 4$, respectively, implies

$$\begin{aligned} \underline{\epsilon}(\mathbf{K}_i^{(2)}) \chi_j^{(n-2)} - \underline{\epsilon}(\mathbf{K}_j^{(2)}) \chi_i^{(n-2)} \\ = \underline{\epsilon}(\mathbf{G}_j) [x_j^b (L_b^{(n-2)} - A_b^{(n)})] - \underline{\epsilon}(\mathbf{G}_i) [x_i^b (L_b^{(n-2)} - A_b^{(n)})] \\ + A_b^{(n-2)} (x_i^b v_j^b - x_j^b v_i^b) \quad (n=2, 3), \end{aligned} \quad (3.44a)$$

$$\begin{aligned} \underline{\epsilon}(\mathbf{K}_i^{(2)}) (\chi_j^{(n-2)} - x_j^b Q_b^{(n-4)}) - \underline{\epsilon}(\mathbf{K}_j^{(2)}) (\chi_i^{(n-2)} - x_i^b Q_b^{(n-4)}) \\ = \sum_{r+s=n-2} \{ \underline{\epsilon}(\mathbf{K}_i^{(r)}) [x_j^b (L_b^{(s)} - A_b^{(s+2)})] \\ - \underline{\epsilon}(\mathbf{K}_j^{(r)}) [x_i^b (L_b^{(s)} - A_b^{(s+2)})] \} \quad (n \geq 4). \end{aligned} \quad (3.44b)$$

Now, taking into account (3.6) and (3.11), it is easy to see that the functions $x_j^b Q_b^{(n)}$ are invariant under translations and behave as vectors under rotations in the same way as the functions $\chi_j^{(n)}$. Hence, and according

to (3.43) and (3.44b), it is always possible to make the following choice:

$$x_j^b Q_b^{(n-2)} = \chi_j^{(n)} \quad (n \geq 2), \quad (3.45)$$

which is equivalent to setting the functions $\chi_j^{(n)}$ ($n \geq 2$) equal to zero in Eqs. (3.39d) and (3.40). On the other hand, the Lagrangian is always defined except for an additive constant and the same also happens with the "partial Lagrangians"; hence, it is always possible to carry out the following transformation:

$$L_b^{(n-2)} \rightarrow L_b^{(n-2)} + A_b^{(n)} \quad (n \geq 2), \quad (3.46)$$

which is equivalent to making the constants $A_b^{(n)}$ ($n \geq 2$) equal to zero in the initial equations (3.39d) and (3.40).

Summarizing the previous results, we can say that Eqs. (3.39d) and (3.40) reduce to the following:

$$\sum_{r+s=n} \pm(\mathbf{K}_j^{(r)}) L^{(s)} = - \sum_{r+s=n-2} \pm(\mathbf{H}^{(r)}) (x_j^b L_b^{(s)}) \quad (n \geq 2), \quad (3.39d')$$

$$\begin{aligned} \pm(\mathbf{K}_i^{(2)}) \chi_j^{(n-2)} - \pm(\mathbf{K}_j^{(2)}) \chi_i^{(n-2)} &= \pm(\mathbf{G}_i)(x_j^b L_b^{(n-2)}) - \pm(\mathbf{G}_j)(x_i^b L_b^{(n-2)}) \\ &+ A_b^{(n-2)} (x_i^b v_j^b - x_j^b v_i^b) \quad (n=2, 3) \end{aligned} \quad (3.40a')$$

$$\sum_{r+s=n-2} \{ \pm(\mathbf{K}_i^{(r)}) (x_j^b L_b^{(s)}) - \pm(\mathbf{K}_j^{(r)}) (x_i^b L_b^{(s)}) \} = 0 \quad (n \geq 4). \quad (3.40b')$$

These formulas will be fundamental in the last section of this paper.

4. NO-INTERACTION THEOREM AND EXPANSION IN $1/c$

As we have said in the Introduction, from a theorem by Currie, Jordan, and Sudarshan⁵ the only PIPS admitting a Lagrangian formulation compatible with their invariance are those such that $\mu_a^i(x_j^b, v_c^k) = 0$, that is, the free particle systems. In this section we will carry out a proof of the theorem which has the double advantage of its great simplicity and its particular adaptation to the analysis of the expansions in $1/c$.

The conditions which allow us to get the no-interaction theorem are (1.5c) and those expressing the invariance of the symplectic form σ (2.2) under the one-parameter groups generated by \mathbf{H} and \mathbf{K}_j , that is, the conditions (2.3) and (3.1) or, equivalently, the set of equations (2.4) and (3.2). After (2.4b) and (3.2b) one easily obtains

$$\frac{\partial \tilde{p}_i^{a'}}{\partial v_i^{a'}} = 0 \quad (a' \neq a). \quad (4.1)$$

A result that, taking into account (2.4c) and (3.2c) respectively, gives the following relations:

$$\frac{\partial \tilde{p}_i^{a'}}{\partial x_i^{a'}} - \frac{\partial \tilde{p}_i^a}{\partial x_i^a} = \frac{\partial \mu^{ak}}{\partial v_i^{a'}} \frac{\partial \tilde{p}_i^a}{\partial v_i^a}, \quad (4.2)$$

$$x_i^{a'} \left(\frac{\partial \tilde{p}_i^{a'}}{\partial x_i^{a'}} - \frac{\partial \tilde{p}_i^a}{\partial x_i^a} \right) + \pm(\mathbf{G}_i) \frac{\partial p_i^a}{\partial v_i^{a'}} - x_i^a \frac{\partial \mu^{ak}}{\partial v_i^{a'}} \frac{\partial \tilde{p}_i^a}{\partial v_i^a} = 0, \quad (4.3)$$

from which one obtains, by introducing the first one in the second,

$$(x_i^{a'} - x_i^a) \frac{\partial \mu^{ak}}{\partial v_i^{a'}} \frac{\partial \tilde{p}_i^a}{\partial v_i^a} = \pm(\mathbf{G}_i) \frac{\partial p_i^a}{\partial v_i^{a'}}. \quad (4.4)$$

On the other hand, taking the derivative of (1.5c) with respect to $v_i^{a'}$, one obtains the following:

$$\begin{aligned} \frac{1}{c^2} (x_j^{a'} - x_j^a) \frac{\partial \mu^{ai}}{\partial x_i^{a'}} \\ = \pm(\mathbf{K}_j) \frac{\partial \mu^{ai}}{\partial v_i^{a'}} + \frac{1}{c^2} x_j^a \pm(\mathbf{H}) \frac{\partial \mu^{ai}}{\partial v_i^{a'}} + \frac{1}{c^2} v_i^a \frac{\partial \mu_j^a}{\partial v_i^{a'}} \\ + \frac{1}{c^2} (2v_j^a - v_j^{a'}) \frac{\partial \mu^{ai}}{\partial v_i^{a'}} + \frac{1}{c^2} (x_j^a - x_{vj}) \frac{\partial \mu_j^k}{\partial v_i^{a'}} \frac{\partial \mu^{ai}}{\partial v_i^k} \\ - \frac{1}{c^2} \delta_{ji} v_i^{ak} \frac{\partial \mu^{ai}}{\partial v_i^{ak}}. \end{aligned} \quad (4.5)$$

From an *exact* point of view, Eq. (4.1) is also valid for the functions p_i^a , so that the right-hand side of (4.4) vanishes and hence we have

$$\frac{\partial \mu_a^i}{\partial v_i^{a'}} = 0, \quad (4.6)$$

because σ is of maximum rank. Taking now (4.6) into (4.5), we get

$$\frac{\partial \mu_a^i}{\partial x_i^{a'}} = 0. \quad (4.7)$$

Equations (4.6) and (4.7) already state that there does not exist interaction among the particles, so the no-interaction theorem can be considered as proven. The vanishing of functions μ_a^i can be proven very easily from conditions (1.5), that express the invariance of the dynamical system under the Poincaré group.

Remark: Actually, it can be shown that relations (4.6) and (4.7) are exclusively a consequence of conditions (2.3) and (3.1), that is, in a strict sense, it is not necessary to use the invariance of the system to conclude in the no interaction of the particles. In order to simplify the calculations we have not followed this method here.

Now let us consider the *approximate* point of view, that is, the one consisting of the study of implications of (4.1), (4.4), and (4.5) on the different orders of approximation in expansions of type:

$$p_i^a = \sum_{n=0}^{\infty} \frac{1}{c^n} p_i^{(n)a}, \quad \mu_a^i = \sum_{n=0}^{\infty} \frac{1}{c^n} \mu_a^{(n)i}. \quad (4.8)$$

At n th order ($n \geq 2$) Eqs. (4.1) and (4.4) give the relations

$$\frac{\partial p_i^{(n-2)a}}{\partial v_i^{a'}} = 0, \quad (4.9)$$

$$(x_j^a - x_j^{a'}) \sum_{r+s=n-2} \frac{\partial \mu_a^{(r)k}}{\partial v_i^{a'}} \frac{\partial p_{a'}^{(r)}}{\partial v_i^{ak}} = \pm(\mathbf{G}_j) \frac{\partial p_{a'}^{(n)}}{\partial v_i^{a'}},$$

so, once the order of approximation is fixed as $n \geq 4$, the following condition must be verified:

$$\frac{\partial \mu_a^{(r)i}}{\partial v_i^{a'}} = 0 \quad (r=0, 1, \dots, n-4) \quad (4.10)$$

having assumed only that the symplectic form σ is of maximum rank at zeroth order. Now, taking into account (4.5), it turns out, after (4.10), that for an order of approximation $n \geq 6$ one also has

$$\frac{\partial \mu_a^{(s)i}}{\partial x_i^{a'}} = 0 \quad (s=0, 1, \dots, n-6) \quad (4.11)$$

From (4.10) and (4.11) one arrives at the conclusion that, beginning with the order of approximation $n \geq 6$, the interaction among the particles in the nonrelativistic limit (classical) vanishes, that is, that in a context of approximation in $1/c$, the no-interaction theorem of Currie, Jordan, and Sudarshan starts to be really effective from order $1/c^6$ on. Hence, one expects to be able to find approximate Lagrangians up to order $n=5$ having a "freeless" classical limit and giving relativistic invariant dynamical systems, those Lagrangians being compatible with the symmetries.

5. APPROXIMATE LAGRANGIANS UP TO ORDER $1/c^4$

Our goal is now to use the results of subsection (B) of Sec. 3 to obtain a family of approximate Lagrangians up to order $1/c^4$ having all the desirable properties, corroborating in this way the conclusions of the preceding section. To make the calculations easier, we will restrict ourselves to the case of *two* particles and we will assume that the classical limit is *Newtonian*, that is,

$$L^{(0)} \equiv \frac{1}{2}m_1v_1^2 + \frac{1}{2}m_2v_2^2 - V(r), \quad (5.1)$$

where m_a is the mass of the particle a , v_a^2 is the square of the modulus of the velocity of this particle, and $V(r)$ is the interaction potential, r being the distance between the particles, that is, with obvious notations:

$$r \equiv (\mathbf{x}^2)^{1/2}, \quad \mathbf{x} \equiv \mathbf{x}_1 - \mathbf{x}_2. \quad (5.2)$$

We will also assume that in the approximate Lagrangian we are looking for, the odd orders do not appear; this is perfectly compatible with all the required conditions.

Taking into account expression (5.1) for $L^{(0)}$, Eqs. (3.38) (zeroth order) yield the following relations:

$$\begin{aligned} F_a^{(0)i} &\equiv m_a \mu_a^{(0)i} = -\frac{\dot{V}}{r} x_{aa}^i, \quad (\circ \equiv \frac{d}{dr}, \quad x_{aa}^i \equiv x_a^i - x_a^i), \\ A_a^{(0)} &\equiv m_a - \eta_a \chi, \quad \chi_j^{(0)} \equiv \chi x_j \quad (\chi = \text{const}; \eta_1 \equiv 1, \eta_2 \equiv -1), \end{aligned} \quad (5.3)$$

which means that the "force" between the particles is of Newtonian type at this order as was expected.

Let us go now to the order $n=2$. According to (3.39a) and (5.1), we have

$$L_a^{(2)} \equiv \frac{1}{2}m_a v_a^2 - \frac{1}{2}V(r) + \eta_a Q(r); \quad (5.4)$$

therefore, taking into account (5.3), relation (3.40a')

holds identically and, on the other hand, Eq. (3.39d') can be written as follows:

$$\begin{aligned} \underline{L}(\mathbf{G}_j) L^{(2)} &= -\underline{L}(\mathbf{K}_j^{(2)}) L^{(0)} - \underline{L}(\mathbf{H}^{(0)})(x_j^b L_b^{(0)}) \\ &= -\left\{ \frac{1}{2} \frac{\dot{V}}{r} [(\mathbf{xv}_1) + (\mathbf{xv}_2)] + \frac{\dot{Q}}{r} [(\mathbf{xv}_1) - (\mathbf{xv}_2)] \right\} x_j \\ &\quad + \left\{ \frac{1}{2} m_1 v_1^2 + \frac{1}{2} V(r) - Q(r) \right\} v_{1j} \\ &\quad + \left\{ \frac{1}{2} m_2 v_2^2 + \frac{1}{2} V(r) + Q(r) \right\} v_{2j}, \end{aligned} \quad (5.5)$$

whose general solution, after (3.39c), is the following:

$$\begin{aligned} L^{(2)} &= \frac{1}{8} m_1 v_1^4 + \frac{1}{8} m_2 v_2^4 + \frac{1}{4} (v_1^2 + v_2^2) V(r) \\ &\quad - \frac{1}{4r} [(\mathbf{xv}_1)^2 + (\mathbf{xv}_2)^2] \dot{V}(r) - \frac{1}{2} (v_1^2 - v_2^2) Q(r) \\ &\quad - \frac{1}{2r} [(\mathbf{xv}_1)^2 - (\mathbf{xv}_2)^2] \dot{Q}(r) + F(r, s, v^2), \end{aligned} \quad (5.6)$$

where F is an arbitrary function of its arguments, and

$$\begin{aligned} \mathbf{v} &\equiv \mathbf{v}_1 - \mathbf{v}_2 \Rightarrow v^2 = (\mathbf{v}\mathbf{v}), \\ s &\equiv \frac{1}{2}(\mathbf{x}\mathbf{v}). \end{aligned} \quad (5.7)$$

Upon introducing (5.1) and (5.6) into (3.39b), one could compute the forces at the order considered.¹⁴

Let us finally deal with the order $n=4$. Recalling (3.39a) it is found that function F is bound to have the following structure:

$$F(r, s, v^2) = B(r) \circ s + E(r) \quad (5.8)$$

so that

$$\begin{aligned} L_a^{(2)} &\equiv \frac{1}{8} m_a v_a^4 + \frac{1}{4} v_a^2 V(r) - \frac{1}{4r} (\mathbf{xv}_a)^2 \dot{V}(r) - \frac{1}{2} \eta_a v_a^2 Q(r) \\ &\quad - \frac{1}{2r} \eta_a (\mathbf{xv}_a)^2 \dot{Q}(r) + \frac{1}{2} (\mathbf{x}_{aa} \cdot \mathbf{v}_a) B(r) + \frac{1}{2} E(r) + \eta_a D(r). \end{aligned} \quad (5.9)$$

Thus, one easily sees that condition (3.40b') holds identically. On the other hand, condition (3.39d') yields the following equation to determine the Lagrangian at fourth order

$$\underline{L}(\mathbf{G}_j) L^{(4)} = -\underline{L}(\mathbf{K}_j^{(2)}) L^{(2)} - \underline{L}(\mathbf{H}^{(0)})(x_j^b L_b^{(2)}), \quad (5.10)$$

where the identity

$$\underline{L}(\mathbf{K}_j^{(4)}) L^{(0)} = -\underline{L}(\mathbf{H}^{(2)})(x_j^b L_b^{(0)}) \quad (5.11)$$

has been used. A straightforward calculation shows that Eq. (5.10) can be written down explicitly as follows:

$$\begin{aligned} \underline{L}(\mathbf{G}_j) L^{(4)} &= \left\{ (\dot{V}/4r) [(\mathbf{xv}_1) v_2^2 + (\mathbf{xv}_2) v_1^2] - (1/4r^2) (\ddot{V} - \dot{V}/r) (\mathbf{xv}_1) (\mathbf{xv}_2) [(\mathbf{xv}_1) + (\mathbf{xv}_2)] - \frac{1}{2} (\dot{V}/r) (\mathbf{v}_1 \mathbf{v}_2) [(\mathbf{xv}_1)^2 + (\mathbf{xv}_2)^2] \right. \\ &\quad + (\dot{Q}/2r) [(\mathbf{xv}_1) v_2^2 - (\mathbf{xv}_2) v_1^2] - (1/2r^2) (\ddot{Q} - \dot{Q}/r) (\mathbf{xv}_1) (\mathbf{xv}_2) (\mathbf{xv}) - (\dot{Q}/r) (\mathbf{v}_1 \mathbf{v}_2) (\mathbf{xv}) + (\dot{E}/2r) [(\mathbf{xv}_1) + (\mathbf{xv}_2)] \\ &\quad - (\dot{D}/r) (\mathbf{xv}) \left. \right\} x_j + \left\{ \frac{3}{8} m_1 v_1^4 + \frac{1}{4} v_1^2 V(r) - \frac{1}{4} (\dot{V}/r) (\mathbf{xv}_1)^2 - \frac{1}{2} v_1^2 Q(r) - (\dot{Q}/2r) (\mathbf{xv}_1)^2 - \frac{1}{2} E(r) - D(r) \right\} v_{1j} \\ &\quad + \left\{ \frac{3}{8} m_2 v_2^4 + \frac{1}{4} v_2^2 V(r) - \frac{1}{4} (\dot{V}/r) (\mathbf{xv}_2)^2 + \frac{1}{2} v_2^2 Q(r) + (\dot{Q}/2r) (\mathbf{xv}_2)^2 - \frac{1}{2} E(r) + D(r) \right\} v_{2j}, \end{aligned} \quad (5.12)$$

whose general solution, taking into account (3.39c), is the following:

$$\begin{aligned} L^{(4)} &= \frac{1}{16} m_1 v_1^6 + \frac{1}{16} m_2 v_2^6 + \frac{1}{16} (v_1^4 + v_2^4) V(r) - \frac{1}{4} (v_1^2 + v_2^2) E(r) + (\dot{E}/4r) [(\mathbf{xv}_1)^2 + (\mathbf{xv}_2)^2] \\ &\quad - (1/8r^2) (\ddot{V} - \dot{V}/r) (\mathbf{xv}_1)^2 (\mathbf{xv}_2)^2 + (\dot{V}/8r) \{ (\mathbf{xv}_1)^2 v_2^2 + (\mathbf{xv}_2)^2 v_1^2 - (\mathbf{v}_1 \mathbf{v}_2) [(\mathbf{xv}_1)^2 + (\mathbf{xv}_2)^2] \} \\ &\quad + (\dot{Q}/4r) \{ (\mathbf{xv}_1)^2 v_2^2 - (\mathbf{xv}_2)^2 v_1^2 - 2(\mathbf{v}_1 \mathbf{v}_2) [(\mathbf{xv}_1)^2 - (\mathbf{xv}_2)^2] \} + (1/24r^2) (\ddot{Q} - \dot{Q}/r) [(\mathbf{xv}_1)^2 - (\mathbf{xv}_2)^2] \end{aligned}$$

$$\times [(\mathbf{xv})^2 - 2(\mathbf{xv}_1)(\mathbf{xv}_2)] - (\dot{D}/2r)[(\mathbf{xv}_1)^2 - (\mathbf{xv}_2)^2] - (D/2)(v_1^2 - v_2^2) + H(r, s, v^2), \quad (5.13)$$

where H is an arbitrary function of its arguments. By introducing now (5.1), (5.6), and (5.13) into (3.39b), it is possible to compute the forces at this order.

In this way we have obtained the most general approximate Lagrangian (except for odd orders which, in fact, are computed trivially) having a Newtonian limit and leading to relativistic invariant dynamical systems (approximate). Moreover, the corresponding Lagrangian formulation is compatible with the invariance under the Poincaré group. On the other hand, (except for the $1/c^5$ order) the approximation obtained is maximum.

By using a standard procedure it is easy to compute the conserved quantities related to the obtained Lagrangian, i. e., energy, momentum, and angular momentum as well as the center of mass position. Since the calculation is obvious, it is not shown here.

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A method for calculation of Regge poles in atomic collisions

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A method for solving the Schrödinger equation is given. It is specially developed for applications in atomic (short wavelength) collisions. The method is also useful for calculating Regge poles, without having to define the potential for complex coordinate. The stability of the method is discussed.

1. INTRODUCTION

Studies of the Regge poles is essential for understanding the behavior of differential and total cross sections in atomic¹⁻⁵ and short wave length collisions.^{6,7} However, there are very few techniques for the calculation of such poles. The main reason for the lack of methods lies in the numerical difficulty connected with solving the Schrödinger equation. Before explaining the details of these difficulties, let us summarize the requirements of such a method: the method should be fast, numerically stable, and straightforward in application.

There are not many cases where the Regge poles are known exactly: They are the Coulomb field,⁸ hard core,⁶ and the potential well.⁷ None of these potentials could even reasonably approximate interaction between the atoms, hence one should resort to numerical techniques. However, before that one should conveniently adapt the appropriate equations.

When solving the Schrödinger equation

$$\psi'' = [V(r) + (\lambda^2 - \frac{1}{4})/r^2 - k^2] \psi = f(r) \psi \quad (1.1)$$

for atoms, the first difficulty comes from the large number of integration steps. Since $f(r)$ is usually large and negative, hence the solution ψ rapidly oscillates, the step length of the numerical integration procedure is small. In such a case the number of steps, hence the accumulation of the numerical error, is noticeable. Therefore, one should not integrate (1.1) since that would considerably slow down the numerical calculation.

Let us explain the source of numerical instabilities. The wavefunction is in the asymptotic region $r \rightarrow \infty$ of the form $\psi = a \exp(ikr) + b \exp(-ikr)$. For an arbitrary complex λ from the first quadrant, the coefficient a is large while b is small.⁹ When integrating (1.1) we therefore find that the solution ψ is approximately $a \exp(ikr)$, to within the numerical error. Since the Regge poles are the complex roots of b in the variable λ , it is clear that we will be unable to determine when the component with $\exp(-ikr)$ is exactly zero.

Two interesting procedures have been proposed to remove this difficulty. One is based on the exact solution of (1.1),⁹ and the other uses the WKB method.¹⁰⁻¹² Several other techniques^{13,14} do not take into account the specific problems of atomic collisions.

Perhaps it would be proper at this place to comment on these two methods. The coordinate-rotation method⁹

is based on the idea that by integrating (1.1) along a convenient path in the complex r plane, the dominant component of ψ becomes subdominant, i. e., we obtain ψ in the asymptotic region having $a \exp(ikr)$ small and $b \exp(-ikr)$ large. In such case it is easy to determine when b is zero.

However, there are major objections to this method. It is obviously not fast, since the wavefunction is integrated. Furthermore, in the complex coordinate plane one solves four coupled equations. It is not numerically stable because of the accumulation of errors due to the large number of integration steps. It is also not straightforward because for the potentials not having simple form,¹⁵ continuation into the complex coordinate plane is not trivial. One should also notice that in the complex r plane the physical picture of interaction is lost, hence it is not easy to deduce what part of the potential curve is responsible for the observed features of scattering cross section. This point is essential for the inversion of the differential cross section procedure.¹⁶

The other method, based on the WKB approximation, also has drawbacks. Perhaps the biggest is the difficulty in understanding the behavior of complex turning points of $f(r)$. Since this requires analytic continuation of $V(r)$ into the complex r plane, the method is also cumbersome in application.

In this article, the problems just mentioned are circumvented by defining a different approach to the Schrödinger equation. Instead of solving (1.1), the equation is transformed to a nonlinear form, the procedure somewhat similar to the method of Calogero,^{17,18} It is shown that solving such an equation is easier, since the basic solution is nonoscillatory, and calculation of the Regge poles is numerically stable. Some very useful approximations are also obtained. The potential does not have to be continued for complex r , therefore the method can also be used when $V(r)$ is tabulated (provided we fit points locally by a polynomial). However, there are two major objections to this method. The derivatives of $V(r)$ should be calculated and the Hankel functions have to be very accurately given.

2. FORMAL THEORY

It can be shown¹⁸ that solving (1.1) provides more information than we actually need for calculation of the phase shifts and the poles of the S matrix. The S

matrix, it was shown,¹⁸ is given by

$$S(\lambda, k) = -\frac{H_{\lambda}^{(2)}(kr_M)}{H_{\lambda}^{(1)}(kr_M)} \left[\frac{H_{\lambda-1}^{(2)}(kr_M)}{H_{\lambda}^{(2)}(kr_M)} + \frac{1}{2kr_M} - \frac{\lambda}{kr_M} - \frac{X}{k} \right] / \left[\frac{H_{\lambda-1}^{(1)}(kr_M)}{H_{\lambda}^{(1)}(kr_M)} + \frac{1}{2kr_M} - \frac{\lambda}{kr_M} + \frac{X}{k} \right], \quad (2.1)$$

where r_M is the value of r from the asymptotic region where the potential is small or zero. The function X is the logarithmic derivative of ψ , and $H_{\lambda}^{(n)}(z)$, $n=1, 2$ are the Hankel functions.¹⁹ Therefore, for a complete determination of the S matrix, only the logarithmic derivative ψ'/ψ is required and not ψ and ψ' explicitly.

The inverse of X , designated by Y , is a solution of the equation

$$Y' = 1 - fY^2, \quad (2.2)$$

which is obtained by taking the derivative of $X=1/Y = \psi'/\psi$ and using (1.1). The difficulties of (1.1) have not been removed by defining (2.2) but they have become even more complex since Y is infinite whenever $\psi' = 0$.

In the next step one defines a transformation on Y such that the oscillations and singularities of Y are explicitly incorporated in the known functions. Such a transformation is¹⁸

$$Y = \frac{1}{f^{1/2}} \tanh(f^{1/2}Z). \quad (2.3)$$

However, here we follow another procedure. The wavefunction ψ is first replaced by $\psi = f^{-1/4}\varphi$, which is in accordance with the WKB approximation.

Therefore, we have for Y

$$Y = 1/(-f'/4f + f^{1/2}/u), \quad (2.4)$$

where $u = \varphi/\dot{\varphi}$ and $d\varphi/d\xi = \dot{\varphi}$. The variable ξ is defined by $d\xi/dr = f^{1/2}$. The equation, which the function u satisfies, is obtained by taking the derivative of (2.4) and using (2.2). We get

$$\dot{u} = 1 - (1+Q)u^2, \quad (2.5)$$

where

$$Q = \frac{1}{4f^2} \left(f'' - \frac{5f'^2}{4f} \right). \quad (2.6)$$

Equations (2.2) and (2.5) explicitly show the symmetry between Y and u because they satisfy the identical equation. We obtain (2.5) by replacing r with ξ and f by $1+Q$, in the equation for Y .

The quantity Q is called the "index of quality" and was first introduced by Kemble.²⁰ Its value is small compared to 1, but near the turning points of f it goes to infinity. However, there is a qualitative difference between this Q and the index of quality defined by Kemble. The index of quality here does not go to zero for $r \rightarrow 0$, as it should. Instead it goes to a finite small number. The difference is in the definition of f in (2.4). Kemble defined f by $f = V + \lambda^2/r^2 - k^2$, while here it is given by (1.1). One might therefore expect difficulties for $r \rightarrow 0$, but it should be pointed out that this method is developed for integrating the Schrödinger equation in the oscillatory region. In the tunneling region near

the origin, one can integrate the equation for Y (or any other) without any difficulties, and when well away from $r=0$, transform to the equation for u . The advantage of (2.6) is that for $r \rightarrow \infty$ the index of quality goes to zero much faster than that defined by Kemble (see the Appendix). Hence, the quantity Q here is primarily defined to be useful in the asymptotic region.

The solution of (2.5) is of a similar behavior as Y . Therefore, we define a new function E , in analogy to Z from (2.3). We have

$$u = \frac{1}{(1+Q)^{1/2}} \tanh(E) \quad (2.7)$$

and the equation for E is

$$\dot{E} = (1+Q)^{1/2} + \frac{\dot{Q}}{4(1+Q)} \sinh(2E) \quad (2.8)$$

or

$$E' = [f(1+Q)]^{1/2} + \frac{Q'}{4(1+Q)} \sinh(2E). \quad (2.9)$$

One uses the inverse of (2.7),

$$E = \frac{1}{2} \ln \frac{1 + (1+Q)^{1/2}u}{1 - (1+Q)^{1/2}u}, \quad (2.10)$$

to obtain E from u .

It is interesting to notice that (2.9) also fails near $Q = -1$ in addition to $f=0$. Therefore, we apply Eq. (2.9) for the case $|Q| < 1$.

3. DISCUSSION OF THE FUNCTION E

Let us now discuss Eq. (2.9). We take that the variables k and λ are real, hence f and Q are real too.

In the oscillatory region we have $f < 0$, therefore the solution E is imaginary and $|\sinh(2E)|$ is less than one. Hence, the first approximation of E is integrated from

$$E'_0 = [f(1+Q)]^{1/2} \quad (3.1)$$

and the solution is nonoscillatory (a similar result is obtained when one integrates the equation for Z ¹⁸). The approximation E_0 is in error to the exact solution by

$$E = E_0 + e \quad (3.2)$$

and to get an estimate of e we replace E in (2.9) by (3.2). If higher than the first powers of e are neglected, the resulting equation for e is linear,

$$e' = -\frac{Q'}{4(1-Q)} [\sin(2E_0) + 2e \cos(2E_0)], \quad (3.3)$$

and the solution, with the initial condition $e=0$ at $r=r_0$, is given by

$$e = -\frac{1}{4} \int_{r_0}^r dr' \frac{Q'}{1-Q} \sin(2E_0) \times \exp\left(-\frac{1}{2} \int_{r'}^r dr'' \frac{Q'}{1-Q} \cos(2E_0)\right). \quad (3.4)$$

In Eq. (3.3) and (3.4) we have replaced E_0 by iE_0 , Q by $-Q$, and e by ie .

The error e is small because Q' is small. Also, since E_0 is large, the integrand in (3.4) rapidly oscillates. The integral (3.4) in average tends to zero, therefore e is small indeed. A nice thing about e is that it contributes to E absolutely. A direct consequence of this is that integrating (2.9) is numerically a stable procedure. Discussion of Z has shown that explicitly.¹⁸

Let us now specify f to be positive and large. The solution E is now real. In the first approximation we can assume that E is small, therefore Eq. (2.9) again reduces to (3.1). We conclude that the solution is positive and rising until reaching such value that the product $\exp(2E) Q'/8$ is comparable to $f^{1/2}$. (When Q' is positive, it is obvious that E is positive and rising without the bounds.) This is usually a large number since $Q'/f^{1/2}$ is small. When E is large and positive, Eq. (2.9) then approximates

$$E'_0 = [f(1+Q)]^{1/2} + \frac{Q'}{8(1+Q)} \exp(2E_0) \quad (3.5)$$

and the solution E_0 is given by

$$\exp(-2E_0) = \exp(-2\xi) \left(\exp(-2E^0) - \frac{1}{4} \int_{r_0}^r \exp(2\xi') \frac{Q'}{1+Q} dr' \right), \quad (3.6)$$

where $\xi = \int_{r_0}^r [f(1+Q)]^{1/2} dr'$ and E^0 is the initial value of E_0 at $r=r_0$.

It is interesting to notice that (3.6) was derived independent of the value of Q , because the accuracy depends essentially on the value of E_0 . There are, however, three cases when $Q' > 0$, which need to be considered: (a) when the integral in the bracket is smaller, (b) when it is equal, (c) when it is greater than $\exp(-2E^0)$. In the first case, the solution E_0 is approximately $E_0 = E^0 + \xi$, therefore it is positive and rising. When the integral equals the first term, the bracket is zero (the second case) and E_0 is infinite, therefore Eq. (2.9) does not have a solution. In the case (c) the solution for E_0 is complex, i. e., shifted from the real axes by $\mp i\pi$ [one can notice from (2.9)/(3.5) that E/E_0 is arbitrary to an imaginary term, which is a multiple of π].

When the integral in (3.6) is negative, the solution for E_0 is always real. It is also interesting to notice that when the integral is much greater than $\exp(-2E^0)$, the solution E_0 does not depend on the initial conditions at $r=r_0$. In this case, we have

$$E_0 \sim \xi - \frac{1}{2} \ln \left(-\frac{1}{4} \int_{r_0}^r \exp(2\xi') \frac{Q'}{1+Q} dr' \right). \quad (3.7)$$

Let us now estimate the error to the solution of (2.9) made by the approximation E_0 . We put

$$E = E_0 + e \quad (3.8)$$

and following the same procedure leading to (3.3) we get the differential equation for e ,

$$e' = \frac{Q'}{2(1+Q)} \left[e \cosh(2E_0) - \frac{1}{4} \exp(-2E_0) \right]. \quad (3.9)$$

The solution of this equation, with the initial condition $e=0$ at $r=r_0$, is

$$e = -\frac{1}{8} \int_{r_0}^r dr' \frac{Q'}{1+Q} \exp(-2E_0) \times \exp \left(\frac{1}{2} \int_{r_0}^r \frac{Q'}{1+Q} \cosh(2E_0) dr' \right). \quad (3.10)$$

The last equation is simplified if $\cosh(x)$ is replaced by the approximate value $\exp(x)/2$. We get

$$e = -\frac{1}{8} \exp(2E_0 - 2\xi) \times \int_{r_0}^r dr' \frac{Q'}{1+Q} \exp(-4E'_0 + 2\xi'), \quad (3.11)$$

where the solution (3.6) was used. Since E_0 is approximately equal to ξ , the result (3.11) shows that the error e is indeed small.

In the conclusion we say that (3.6) can be used as the approximate solution of E , but the error e should be evaluated before that. It should also be borne in mind that (3.6) is valid if E_0 is large.

So far the assumption was that λ and k are real. Let us now make λ complex in the first quadrant. In the previous analysis of E , we have nowhere used f explicitly (only through Q), therefore we can apply that discussion to this case as well, however, with certain modifications. Thus for example, the approximation (3.1) works if the real part of E is small by absolute value, and the approximation (3.6) works when the real part of E is large. In both cases one should calculate e to have an exact estimate of the accuracy of the approximation E_0 .

Very often Eq. (2.9) is solved numerically. The analysis of the error e ¹⁸ shows that the numerical procedure is stable to the variations of the step length. A modestly advanced numerical algorithm would give good results. However, care should be taken when being in the vicinity of a singular point of E .

4. CALCULATION OF THE S MATRIX

The S matrix is given by (2.1). It was shown, in the previous section, how to calculate X . Let us now show how one uses this result to calculate the S matrix. From (2.7) and (2.4) we have

$$X = -\frac{f'}{4f} + \frac{[f(1+Q)]^{1/2}}{\tanh(E)}. \quad (4.1)$$

For complex λ , the real part of E can be large. Therefore, we replace $\tanh(E)$ by

$$\frac{1}{\tanh(R+iI)} = 1 + \frac{2 \exp(-R)}{\exp(R) + \exp(-R)} \frac{1 - i \tan(I)}{\tanh(R) + i \tan(I)} \quad (4.2)$$

and the function X is

$$X = -\frac{f'}{4f} + [f(1+Q)]^{1/2} + [f(1+Q)]^{1/2} \frac{2 \exp(-2R)}{\exp(-2R) + 1} \frac{1 - i \tan(I)}{\tanh(R) + i \tan(I)}, \quad (4.3)$$

where $R = \text{Re}(E)$ and $I = \text{Im}(E)$.

Let us pay attention to $H_{\lambda-1}^{(n)}/H_{\lambda}^{(n)}$, $n=1, 2$. It is shown in the Appendix that the ratio of Hankel functions can be approximated by

$$\frac{H_{\lambda-1}^{(n)}(z)}{H_{\lambda}^{(n)}(z)} = \frac{\lambda}{z} - \frac{1}{2z} - \frac{f_0'}{4f_0} - (-)^n [f_0(1+Q_0)]^{1/2} + O(Q_0'/4), \quad (4.4)$$

where

$$f_0 = \frac{\lambda^2 - \frac{1}{4}}{z^2} - 1$$

and

$$Q_0 = \frac{\lambda^2 - \frac{1}{4}}{4} \frac{\lambda^2 - \frac{1}{4} - 6z^2}{(\lambda^2 - \frac{1}{4} - z^2)^3}. \quad (4.5)$$

Therefore, the denominator of (2.1) is

$$D = \eta(z) + O\left(\frac{Q'}{4}\right) - \frac{2}{k} [f(1+Q)]^{1/2} \times \frac{\exp(-2R)}{\exp(-2R)+1} \frac{1-i \tan(I)}{\tanh(R)+i \tan(I)}, \quad (4.6)$$

where we have defined the error η by

$$\eta(z) = \frac{f'}{4kf} - \frac{f_0'}{4f_0} - \frac{1}{k} [f(1+Q)]^{1/2} + [f_0(1+Q_0)]^{1/2}. \quad (4.7)$$

Usually, the errors η and $O(Q'/4)$ are small, therefore the denominator D is mainly determined by the last term

$$D \sim -\frac{2}{k} [f(1+Q)]^{1/2} \frac{\exp(-2R)}{\exp(-2R)+1} \frac{1-i \tan(I)}{\tanh(R)+i \tan(I)}. \quad (4.8)$$

This is the case when λ is real or complex with a small imaginary part. However, when R is large, then the last term in D competes in magnitude with $O(Q'/4)$ and η . We distinguish now two cases: (a) when η is larger or equal compared to $O(Q'/4)$; (b) η is much smaller than $O(Q'/4)$. In the first case it means that D , hence $S(\lambda, k)$, depends on the form of the potential at $r=r_M$, since η is potential dependent. We can do two things to remove this difficulty. One is to take r_M further out to make $V(r)$ even smaller. The other possibility is discussed in the Conclusion.

In the case (b) the term η can be neglected and D is given by (4.8) plus the remainder $O(Q'/4)$.

Using (4.4) in the numerator of (2.1), we have

$$N = -2[f_0(1+Q_0)]^{1/2} \times \left(1 + \frac{\exp(-2R)}{\exp(-2R)+1} \frac{1-i \tan(I)}{\tanh(R)+i \tan(I)}\right), \quad (4.9)$$

where the errors η and $O(Q'/4)$ were neglected. They are always much smaller than the leading term $f_0^{1/2}$, provided that r_M is in the asymptotic region.

For almost real λ the numerator N is

$$N = -[f_0(1+Q_0)]^{1/2} \frac{\exp(E)}{\sinh(E)}, \quad (4.10)$$

hence the S matrix (2.1) is

$$S(\lambda, k) \sim -\frac{H_{\lambda}^{(2)}(kr_M)}{H_{\lambda}^{(1)}(kr_M)} \exp(+2E). \quad (4.11)$$

However, when R is large the second term in N is small and we have for the S matrix

$$S(\lambda, k) = \frac{H_{\lambda}^{(2)}(kr_M)}{H_{\lambda}^{(1)}(kr_M)} \frac{2[f_0(1+Q_0)]^{1/2}}{D}, \quad (4.12)$$

where D is given by (4.8) plus the term $O(Q'/4)$.

The Regge poles are now calculated from the equation $D=0$ (4.13)

for complex λ . However, the procedure is not as straightforward as one might expect. We will shortly come to this point, but we will now discuss the last equation.

For a complex angular momentum, with small imaginary part, the approximation (4.8) works well. However, Eq. (4.13) can only have a solution if $R \rightarrow \infty$, therefore, in a small neighborhood of the almost real Regge pole, the approximation (4.8) is no longer valid and $O(Q'/4)$ and η should be calculated. Usually, this is not the case. Namely, in such a close vicinity of the Regge pole, where O and η are becoming significant, the value of λ is very near to the root of Eq. (4.13). Therefore, in practice we can take that value for the Regge pole.

For the Regge poles away from the real axes, the approximation (4.8) is no longer useful and one has to take $O(Q'/4)$ into account. However, one should inspect before that, whether η is small. Otherwise, r_M should be taken further out.

5. SOURCES OF INACCURACY

There are two major sources of the inaccurate results: numerical and inherent in the theory. The two are mutually interwoven, because the equations resulting from the theory have to be solved numerically. We are not going into the details of the numerical procedures for solving the equations, because something similar was done for the function Z ,¹⁸ defined by (2.3). In short, Eq. (2.9) is convenient for solving numerically since the basic solution is nonoscillatory.

More important are the sources of inaccuracy directly incorporated in the theory. For this reason, we have to analyze every step leading to the final result, the S matrix.

Let us first discuss the case when λ is almost real. Solving Eq. (2.9) is no problem in the region where $|Q| < 1$. However, it would perhaps be more convenient to use (2.9) in the oscillatory region while integrating (2.2) in the tunneling region and around the turning points of f . The discussion following (3.6) showed that E can have logarithmic singularities in the tunneling region, but Y can only have one first order pole. Integration of (2.2), therefore, gives better chances of success. Anyhow, one should not have difficulties in obtaining the accurate S matrix.

A very serious source of inaccuracy is cancelation of the significant figures. This occurs in (4.6) for a complex λ with a large imaginary part. Let us see that more closely. When R is large, then D is

$$D \sim O\left(\frac{Q'}{4}\right) - \frac{2}{k} [f(1+Q)]^{1/2} \exp(-2E), \quad (5.1)$$

where we have neglected the term η . Let us use (3.6) as an estimate for E , in which case D becomes

$$D \sim O\left(\frac{Q'}{4}\right) - \frac{2}{k} [f(1+Q)]^{1/2} \times \left(\exp(-2E^0) - \frac{1}{4} \int_{r_0}^r \exp(2\xi') \frac{Q'}{1+Q} dr' \right) \exp(-2\xi). \quad (5.2)$$

Since the real part of ξ is large and positive, the integral in D is dominated by the value of the integrand near the upper limit. By comparing the leading term of the integral from (5.2) with $O(Q'/4)$ from the Appendix, it follows that these terms cancel. If $\exp(-2E^0)$ is much smaller than the value of the integral, there will be cancellation of the numerically significant figures of E . By putting the leading term of $O(Q'/4)$ into Eq. (5.1) we conclude that Eq. (2.9) gives accurate results for the S matrix if in the asymptotic region we have the inequality

$$\exp(-2R) > \left| \frac{Q'}{8f^{1/2}} \right|. \quad (5.3)$$

However, when the approximate equality holds, then a cancellation in D is expected. Hence the region of the λ plane beyond this point cannot be reached by the solution of (2.9). It is the "forbidden region" of (2.9).

One should notice that when the terms in (5.1) cancel, the error η becomes an important contribution to the S matrix and r_M should be taken further out.

Another serious source of inaccuracy is calculating $O(Q'/4)$ from (4.4). The left-hand side is calculated exactly (e.g., from the asymptotic expansion of the Bessel functions¹⁹) and from that the right-hand side, without $O(Q'/4)$, is subtracted. The remainder is O . Therefore, if the right-hand side of (4.4) accurately represents the ratio of the Hankel functions, say to eight significant figures, then the Hankel functions should be accurately given to 12 figures if the final result is expected to be accurate to four figures. Such a difficulty appears when the Regge poles with large imaginary part are calculated, when the representation (4.8) is no longer accurate. However, this problem can be circumvented since the properties of the Hankel functions are very well understood. Also, O is independent of the form of the potential, therefore, we assume that calculating O is a standard procedure, but not unimportant.

A source of inaccuracy is also calculating η . It is a minor difficulty, because when the potential is much smaller than the centrifugal term, any function of f can always be expanded in the powers of V/f_0 .

6. GENERALIZATION OF THE THEORY

Let us have a look again at the steps leading to the equation for E . We have a function Y satisfying the equation

$$Y' = 1 - fY^2, \quad (6.1)$$

where Y was given as the ratio $Y = \psi/\psi'$. Then, we defined $\psi = f^{-1/4}\varphi$ and replaced r by $\xi = \int_{r_0}^r f^{1/2} dr$, to obtain an equation for u , defined by $u = \varphi/\varphi'$,

$$\ddot{u} = 1 - (1+Q)u^2, \quad (6.2)$$

where now the derivative is with respect to the variable ξ . The index of quality Q is defined by (2.6). Formally, Eq. (6.2) is identical to (6.1) except that $1+Q$ plays the role of f and ξ is the new coordinate. Let us now repeat the steps, with (6.2) being now the "input," i.e., we define $\varphi = (1+Q)^{-1/4}\omega$ and $\bar{\xi} = \int_{r_0}^r (1+Q)^{1/2} d\xi'$. The equation for $v = \omega/\omega'$ is

$$\ddot{v} = 1 - (1+Q)v^2, \quad (6.3)$$

where the asterisk is the derivative with respect to $\bar{\xi}$ and

$$\underline{Q} = \frac{1}{4(1+Q)^2} \left(\ddot{\bar{Q}} - \frac{5}{4(1+Q)} (\dot{\bar{Q}})^2 \right). \quad (6.4)$$

For v we define \underline{E} by the relationship

$$v = \frac{1}{(1+Q)^{1/2}} \tanh(\underline{E}), \quad (6.5)$$

and the equation which \underline{E} satisfies is

$$\ddot{\underline{E}} = (1+Q)^{1/2} + \frac{\ddot{\bar{Q}}}{4(1+Q)} \sinh(2\underline{E}) \quad (6.6)$$

or

$$\underline{E}' = [f(1+Q)(1+Q)]^{1/2} + \frac{Q'}{4(1+Q)} \sinh(2\underline{E}). \quad (6.7)$$

The new index of quality \underline{Q} is now given in terms of the r derivatives as

$$\underline{Q} = \frac{1}{4f(1+Q)^2} \left(-\frac{f'}{2f} Q' + Q'' - \frac{5}{4(1+Q)} (Q')^2 \right). \quad (6.8)$$

By using the transformations made on the way to v , we can also find the relationship with X , which is

$$X = -\frac{f'}{4f} - \frac{Q'}{4(1+Q)} + \frac{[f(1+Q)]^{1/2}}{v}. \quad (6.9)$$

The formal derivative of Eq. (6.7) can be repeated indefinitely and the result is always an equation of the type (2.9). The leading term of such an equation is

$$F_n = [f(1+Q_1)(1+Q_2) \cdots (1+Q_n)]^{1/2} \quad (6.10)$$

and Q_n is defined by

$$Q_n = \frac{1}{4(1+Q_{n-1})^2} \left[\frac{d^2 Q_{n-1}}{d\xi_{n-2}^2} - \frac{5}{4(1+Q_{n-1})} \left(\frac{dQ_{n-1}}{d\xi_{n-2}} \right)^2 \right], \quad (6.11)$$

where

$$\xi_{n-2} = \int_{r_0}^r F_{n-2}^{1/2} dr'. \quad (6.12)$$

Therefore, Eq. (6.7) brings nothing new into our previous discussion of (2.9) except that with each step, as it will be shown shortly, we get more information about the S matrix. Whatever has been said about (2.9) applies equally well to (6.7) and all the subsequent equations. However, at each step Q_n gets more complicated and also higher derivatives of f are required.

An estimate of O , introduced in (4.6), brings more light onto the purpose of going from (2.9) to (6.7) and further. We will show that Eq. (6.7) gives more infor-

mation about the "forbidden region," discussed in Sec. 5.

Let us firstly prove that a general transformation from X to u_n is of the form

$$X = -\frac{f'}{4f} - \frac{Q_1'}{4(1+Q_1)} - \dots - \frac{Q_n'}{4(1+Q_n)} + \frac{F_n}{u_n}, \quad (6.13)$$

where $Q_1 = Q$, $Q_2 = \underline{Q}$ and F_n is given by (6.10). The equation for u_n is

$$\dot{u}_n = 1 - (1 + Q_{n+1}) u_n^2, \quad (6.14)$$

where the derivative is with respect to $\xi_n = \int^r F_n dr'$.

We prove this by total induction. It is obvious that (6.13) and (6.14) are valid for $n=1$. Now, for a general n , we make the identical transformation leading to (6.9). Namely, we define $u_n = \varphi_n / \dot{\varphi}_n$ and replace φ_n by $\varphi_n = (1 + Q_{n+1})^{-1/4} \omega_n$ to obtain

$$\frac{1}{u_n} = -\frac{\dot{Q}_{n+1}}{4(1+Q_{n+1})} + (1 + Q_{n+1})^{1/2} \frac{\dot{\omega}_n^*}{\omega_n}, \quad (6.15)$$

where now the asterisk is a derivative with respect to ξ_{n+1} . We put relationship (6.15) into (6.13) and get

$$X' = -\frac{f'}{4f} - \frac{Q_1'}{4(1+Q_1)} - \dots - \frac{Q_{n+1}'}{4(1+Q_{n+1})} + \frac{F_{n+1}}{u_{n+1}}, \quad (6.16)$$

where we have used the property that

$$F_n \frac{d}{d\xi_n} = \frac{d}{dr}.$$

A formal derivation of the equation for u_{n+1} , by using (6.14) and (6.15), leads to

$$\dot{u}_{n+1} = 1 - (1 + Q_{n+2}) u_{n+1}^2, \quad (6.17)$$

where

$$Q_{n+2} = \frac{1}{4(1+Q_{n+1})^2} \left(\overset{\circ}{Q}_{n+1} - \frac{5}{4(1+Q_{n+1})} (\overset{\circ}{Q}_{n+1})^2 \right). \quad (6.18)$$

We have obtained the equations identical to (6.13) and (6.14), therefore, we have proved our statement. By repeated transformations of the original equation for X we can get (6.13), where u_n is the solution of (6.14).

Let us now estimate the remainder, defined by

$$\frac{H_{\lambda}^{(1)}(z)}{H_{\lambda}^{(1)}(z)} = \frac{\lambda}{z} - \frac{1}{2z} - \frac{f_0'}{4f_0} - \frac{Q_1'}{4(1+Q_1)} - \dots - \frac{Q_n'}{4(1+Q_n)} + F_{0n}(1+Q_{0n+1})^{1/2} + O_n, \quad (6.19)$$

where $Q_{01}(z) = Q_0(z)$ and $z = kr$.

From the equation for u_n , it is easily proved that φ_n , defined by $u_n = \varphi_n / \dot{\varphi}_n$, is the solution of

$$\overset{\circ}{\varphi}_n = (1 + Q_{n+1}) \varphi_n. \quad (6.20)$$

As in the Appendix, Eq. (6.20) is solved by iterating the appropriate integral equation. Following the same procedure, this equation is

$$\varphi_n = \exp(\xi_n) + \int_{\infty}^{\xi_n} \sinh(\xi_n - \xi_n') Q_{0n+1} \varphi_n d\xi_n' \quad (6.21)$$

which gives, to the second order in Q_{0n+1} , for the ratio

$$\frac{\dot{\varphi}_n}{\varphi_n} = 1 + \exp(-2\xi_n) \int_{\infty}^{\xi_n} \exp(2\xi_n') Q_{0n+1} d\xi_n' \quad (6.22)$$

or

$$\frac{\varphi_n'}{\varphi_n} = (1 + Q_{0n+1}/2 + Q_{0n+1}'/(4F_{0n})) F_{0n}. \quad (6.23)$$

Since ψ is related to φ_n by the relationship $\psi = F_{0n}^{-1/2} \varphi_n$, which is easily proved by forming the logarithmic derivative of ψ and comparing it with the right-hand side of (6.13), we obtain

$$\frac{\psi'}{\psi} \sim -\frac{f_0'}{4f_0} - \frac{Q_{01}'}{4(1+Q_{01})} - \dots - \frac{Q_{0n}'}{4(1+Q_{0n})} + F_{0n} + F_{0n} Q_{0n+1}/2 + Q_{0n+1}'/4, \quad (6.24)$$

which is equal to (6.19) with the remainder being

$$O_n = Q_{0n+1}'/4. \quad (6.25)$$

Let us estimate the order of magnitude of (6.25) in the asymptotic region for $z \gg |\lambda|$. Such an estimate is important since it is not obvious that the repeated transformation procedure of the type (6.15) will converge. For that, we firstly develop Q_{0n} in the inverse power series of z , and calculate the leading term.

The z derivative representation of Q_{0n+1} is

$$Q_{0n+1} = \frac{1}{4F_{0n-1}^2} \left(-\frac{(F_{0n-1}^2)'}{2F_{0n-1}^2} Q_{0n}' + Q_{0n}'' - \frac{5}{4} (Q_{0n}')^2 \right), \quad (6.26)$$

where Q_{0n} was neglected compared to 1. Since $F_{0n-1}^2 = -1$ and the leading term of $(F_{0n-1}^2)'$ is

$$(F_{0n-1}^2)' \sim -2 \frac{\lambda^2 - \frac{1}{4}}{z^3}, \quad (6.27)$$

we have for Q_{0n+1}

$$Q_{0n+1} \sim -\frac{1}{4} \left(-\frac{\lambda^2 - \frac{1}{4}}{z^3} Q_{0n}' + Q_{0n}'' - \frac{5}{4} (Q_{0n}')^2 \right). \quad (6.28)$$

Let us assume that $Q_{0n} \sim z^{-m}$. Then the most dominant term in (6.28) comes from the second derivative of Q_{0n} , therefore

$$Q_{0n+1} \sim -\frac{1}{4} Q_{0n}'' \quad (6.29)$$

The initial condition at $n=1$, for the last equation, is (see the Appendix) $Q_{01} = 3(\lambda^2 - \frac{1}{4})/(2z^4)$. We solve Eq. (6.29) by using the ansatz $Q_{0n} = \alpha_n z^{-2n-2}$, where the coefficients α_n are obtained from

$$\alpha_{n+1} = -\frac{1}{4} \alpha_n (2n+2)(2n+3) \quad (6.30)$$

with the initial condition $\alpha_1 = 3(\lambda^2 - \frac{1}{4})/2$. The solution is

$$\alpha_{n+1} = (-1)^n \frac{(2n+3)!}{4^{n+1}} (\lambda^2 - \frac{1}{4}) \quad (6.31)$$

or

$$Q_{0n+1} \sim (-1)^n \frac{(2n+3)!}{4^{n+1}} (\lambda^2 - \frac{1}{4}) z^{-2n-4}. \quad (6.32)$$

Therefore, the remainder is

$$O_n = (-1)^{n+1} \frac{(2n+4)!}{4^{n+2}} (\lambda^2 - \frac{1}{4}) z^{-2n-5}. \quad (6.33)$$

It is obvious, because of the factorial in the numera-

tor, O_n is not going to zero for large n , hence, the procedure cannot be repeated indefinitely. The series (6.24) is of the asymptotic expansion nature. However, since we can arbitrarily choose z , the series converges in the limit $z \rightarrow \infty$.

For $n=1$, the remainder is

$$\underline{O} = O_1 = \frac{45}{4} \frac{(\lambda^2 - \frac{1}{4})}{z^7}, \quad (6.34)$$

which is several orders of magnitude smaller than $O(Q'/4)$, if z is large. Therefore, the representation of the ratio of Hankel functions is more accurately given by (6.11) than (4.4). However, calculation of the remainder (6.34) is more difficult than before.

The inequality (5.3) determines the boundary in the λ plane beyond which the calculation of the Regge poles is not possible. The similar inequality applied in this case shows that solving (6.7) is "pushing" that boundary towards larger $\text{Im}(\lambda)$ and $\text{Re}(\lambda)$. A part of the λ plane, which was unknown to (2.9) can be reached by (6.7), and the procedure is stable numerically since the only source of inaccuracy comes from calculating (6.34) and η . The procedure can be systematically applied by going to a general Q_n , defined by (6.11). However, one should be careful because the resulting series is asymptotic

7. ONE EXAMPLE

Let us show practically how the method works and compare the results with the known solution. The problem should be specific of the short wave collisions but not very complex so that we loose the main idea of the paper. It should also incorporate all the details of the previous discussion.

Such an example is scattering on the impenetrable sphere,⁶ when the potential $V(r)$ is

$$V(r) = \begin{cases} \infty, & r \leq r_0 \\ 0, & r > r_0. \end{cases} \quad (7.1)$$

It can be shown that the poles are complex roots of $H_\lambda^{(1)}(kr_0)$ in the variable λ . For large values of kr_0 , we have approximately⁶

$$\lambda_n \ln \frac{\lambda_n + (\lambda_n^2 - z_0^2)^{1/2}}{z} - (\lambda_n^2 - z^2)^{1/2} = i(n - 1/4)\pi, \quad (7.2)$$

where $z = kr_0$. Although this example is simple, for its solution we should use all the essential points of the theory. A more complicated example would not give more insight into the understanding of the theory. With $V(r)$ being different than zero at $r = r_M$, the error η , defined in (4.7), should be taken into account. This, however, does not introduce additional difficulties. Extensive calculations on the Regge representation of the scattering amplitude has been made,¹ and this theory was used for obtaining the Regge poles. The results show that calculation of the Regge poles by this method is also very practical.

Let us also compare the residues, given approximately by⁶

$$\text{Res}(S_n) = \frac{\lambda_n}{2[i(n - 1/4)\pi + (\lambda_n^2 - z^2)^{1/2}]} \quad (7.3)$$

with the ones given by this theory. By definition,

$$\text{Res}(S_n) = \lim_{\lambda \rightarrow \lambda_n} (\lambda - \lambda_n) S(\lambda, k) \quad (7.4)$$

and after using (2.1), we obtain

$$\text{Res}(S_n) = \frac{4i}{\pi k r_M} \frac{1}{[H_{\lambda_n}^{(1)}(k r_M)]^2} \frac{1}{\partial D / \partial \lambda_n}. \quad (7.5)$$

The derivative of D was calculated numerically.

Equation (2.9) was integrated using a standard computer package.²¹ When E could not produce the results, the more accurate version of (2.9) was used, i. e., the function \underline{E} was integrated from (6.7). The results obtained by integrating \underline{E} are designated by an asterisk.

The Regge poles were calculated from (4.13), at two different energies. The results are given in Table I, and they are compared with the approximate ones, given by (7.2). In Table I we can also compare the residues calculated from (7.3) and (7.5). Bearing in mind that formulas (7.2) and (7.3) are approximate, the agreement is very good.

8. CONCLUSION

A method was described for the calculation of the Regge poles, suitable for the applications in atomic (short wavelength) collisions. Its main feature is that the results are obtained from the potential defined on the real axis only. However, the derivatives of the potential should be calculated instead.

Some very useful approximations were made [e. g., (3.6)], being of great help if the Regge poles with a large imaginary part are calculated. It was also proved that for the Regge poles of this type, the only difficulty is calculating the remainder O_n , but knowing the properties of the Hankel functions, it can be overcome with ease.

TABLE I. The Regge poles and residues for (7.1). The columns designated by N and E are the results obtained from (7.2) and (4.13), respectively. The asterisk indicates that the numbers were obtained by integrating the equation for \underline{E} .

$k^2 = 10$	N	E	
$n = 1$	4.4805 + i2.4070 0.3497 - i0.1824	4.4874 + i2.4275 0.3475 - i0.1788	λ_n Res(S)
$n = 2$	5.4469 + i4.3198 0.2737 - i0.1342	5.4481 + i4.3281 0.2736 - i0.1328	λ_n Res(S)
$n^* = 3$	6.2190 + i5.9293 0.2419 - i0.1137	6.2195 + i5.9348 0.2402 - i0.1115	λ_n Res(S)
$n^* = 4$	6.8921 + i7.3861 0.2231 - i0.1014	6.8921 + i7.3902 0.2237 - i0.1011	λ_n Res(S)
$k^2 = 100$			
$n = 1$	11.9593 + i3.4814 0.4989 - i0.2739	11.9729 + i3.5088 0.4922 - i0.2695	λ_n Res(S)
$n = 2$	13.4178 + i6.1845 0.3833 - i0.2034	13.4218 + i6.1943 0.3855 - i0.2033	λ_n Res(S)
$n^* = 3$	14.5906 + i8.4245 0.3347 - i0.1730	14.5751 + i8.4382 0.3331 - i0.1727	λ_n Res(S)

Before concluding, let us comment on the point only mentioned in Sec. 4. The error η , defined by (4.7), asymptotically goes to zero not faster than $V(r)$. On the other hand, the remainder O_n , given by (6.33), goes to zero as some inverse power of r . Therefore, the potential $V(r)$ should decay faster for the theory of Sec. 4 to be applicable. Namely, we have assumed that η is always smaller than O_n , and in the case when it is not, r_M is taken further out to the asymptotic region. It is obvious that this cannot be achieved if $V(r) \sim r^{-s}$ for $r \rightarrow \infty$ because for all r_M , η is always larger than the remainder O_n . Hence, the conclusion is that the S matrix (therefore the Regge poles) depends on the form of the potential at $r=r_M$. One can do two things to overcome the difficulty: either r_M is taken to infinity so that the form (4.8) is used for the S matrix, or define a cut off potential at some $r=r_M^0$.¹⁸ In the first case, the solution is not practical since integrating (2.9) to such a large value of r is not feasible. Defining the cutoff potential requires a little more attention. It has been shown that by setting the value of $V(r)$ to zero beyond some $r=r_M^0$, the scattering amplitude does not noticeably change.¹⁸

On the other hand, each Regge pole with a large imaginary part depends on the r_M^0 , as it was shown in Sec. 4. Such poles has interpretation in terms of the surface waves, but only a multitude of them give rise to an experimentally observed quantity, e.g., the differential cross section. Therefore, a single pole may depend on r_M^0 , but the contribution of all poles to the scattering amplitude is independent of r_M^0 . To conclude, dependence of the Regge poles on r_M^0 does not *a priori* mean that the cutting off potential is wrong. It means that various locations of the poles produce one observed differential cross section.

APPENDIX

A special case of (1.1) is when the potential is identical to zero. If the boundary conditions of ψ is either the incoming or outgoing plane wave at infinity, then the two solutions of (1.1) are¹⁹

$$\psi_1 = z^{1/2} H_\lambda^{(1)}(z), \quad \psi_2 = z^{1/2} H_\lambda^{(2)}(z), \quad (A1)$$

where $H_\lambda^{(n)}(z)$ are the Hankel functions, and $z=kr$. The logarithmic derivative of ψ_n is therefore

$$X_n = \frac{\psi_n'}{\psi_n} = \frac{1}{2z} - \frac{\lambda}{z} + \frac{H_\lambda^{(n)'}(z)}{H_\lambda^{(n)}(z)}, \quad n=1, 2, \quad (A2)$$

where we have used the recurrence relation for the Hankel functions.¹⁹

Let us replace ψ_n by

$$\psi_n = f_0^{-1/4} \varphi_n, \quad (A3)$$

where

$$f_0 = \frac{\lambda^2 - \frac{1}{4}}{z^2} - 1 \quad (A4)$$

and put it into Eq. (A2). We get

$$X_n = -\frac{f_0'}{4f_0} + f_0^{1/2} \frac{\varphi_n'}{\varphi_n}, \quad (A5)$$

where the derivative of φ_n is with respect to $\xi = \int^r f_0^{1/2} dz'$.

It can be shown from (A5) and (2.2) that φ_n satisfies the equation

$$\overset{\circ}{\varphi}_n = (1 + Q_0) \varphi_n, \quad (A6)$$

where

$$Q_0 = \frac{\lambda^2 - \frac{1}{4}}{4} \frac{\lambda^2 - \frac{1}{4} - 6z^2}{(\lambda^2 - \frac{1}{4} - z^2)^3} \quad (A7)$$

is the index of quality for the free waves. In the asymptotic region $z \rightarrow \infty$, Q_0 goes to zero as

$$Q_0 \sim \frac{3(\lambda^2 - \frac{1}{4})}{2z^4}. \quad (A8)$$

It is interesting to notice that the index of quality defined by Kemble²⁰ goes to zero only as $Q_0 \sim -1/(4z^2)$.

Since Q_0 is small for large z , it is a convenient quantity for developing the solution of (A6) in the power series

$$\varphi_n = a + bQ_0 + cQ_0^2 + \dots \quad (A9)$$

This is done by transforming (A6) into an integral equation form. It can be shown, by taking derivatives of φ_n , that

$$\varphi_n = \exp(\pm \xi) + \int_{\infty}^{\xi} \sinh(\xi - \xi') Q_0 \varphi_n d\xi' \quad (A10)$$

satisfies the original differential equation. The advantage of (A10) is twofold: Firstly, the boundary condition at infinity is directly incorporated in the equation, and secondly, the iteration of the equation produces a series of the type (A9), which is absolutely convergent for a finite Q_0 .²² The variable ξ can be calculated explicitly, but this is not essential for our discussion. One should be careful, though, to correctly define ξ for large r , so that the behavior of (A10) should have the same phase as $H_\lambda^{(n)}(z)$.

The plus sign in (A10) corresponds to the outgoing waves, hence ψ_1 , and the minus sign to the incoming waves.

The first iteration of (A10) is

$$\varphi_n = \exp(\pm \xi) + \int_{\infty}^{\xi} \sinh(\xi - \xi') Q_0 \exp(\pm \xi') d\xi', \quad (A11)$$

and if in the interval $\xi < \xi' < \infty$, Q_0 is small this representation of φ_n is accurate to the order Q_0^2 . The derivative of (A11), with respect to ξ , is

$$\overset{\circ}{\varphi}_n = \pm \exp(\pm \xi) + \int_{\infty}^{\xi} \cosh(\xi - \xi') Q_0 \exp(\pm \xi') d\xi' \quad (A12)$$

so that we can now form the ratio $\overset{\circ}{\varphi}_n/\varphi_n$. Since the assumption was that $|Q_0| \ll 1$, the inverse of φ_n is developed in the power series of Q_0 , giving

$$\frac{\overset{\circ}{\varphi}_n}{\varphi_n} = \pm 1 + \exp(\mp 2\xi) \int_{\infty}^{\xi} \exp(\pm 2\xi') Q_0 d\xi' \quad (A13)$$

to the second order of Q_0 . The last integral can be partially integrated and we obtain

$$I = \exp(\mp 2\xi) \int_{\infty}^{\xi} \exp(\pm 2\xi') Q_0 d\xi' = \pm \frac{Q_0}{2} + \frac{Q_0'}{4f_0^{1/2}} \pm \frac{\exp(\mp 2\xi)}{4} \int_{\infty}^{\xi} \exp(\pm 2\xi') \frac{1}{f_0^{1/2}} \left(\frac{Q_0'}{f_0^{1/2}} \right)' d\xi', \quad (A14)$$

where it was taken into account that $Q_0 \rightarrow 0$ for $z \rightarrow \infty$. Since the last term is much smaller than the first two, and this is the case when $z \gg |\lambda|$, the ratio (A13) is

$$\frac{\overset{\circ}{\varphi}_n}{\varphi_n} = \pm 1 \pm \frac{Q_0}{2} + \frac{Q_0'}{4f_0^{1/2}}. \quad (\text{A15})$$

If we put this result in (A5) and then in (A2), an approximation of the ratio of Hankel functions is obtained,

$$\frac{H_{\lambda-1}^{(n)}(z)}{H_{\lambda}^{(n)}(z)} = -\frac{1}{2z} + \frac{\lambda}{z} - \frac{f_0'}{4f_0} - (-)^n \frac{1+Q_0}{2} + O\left(\frac{Q_0'}{4}\right). \quad (\text{A16})$$

The procedure can be repeated for (A13), but now taking into account higher powers of Q_0 . The next leading term from the resulting power series is $f_0^{1/2}Q_0^2/4$, and in general, we notice that the terms with Q_0^n , form a power series for the function $(1+Q_0)^{1/2}$, therefore (A16) becomes

$$\frac{H_{\lambda-1}^{(n)}(z)}{H_{\lambda}^{(n)}(z)} = -\frac{1}{2z} + \frac{\lambda}{z} - \frac{f_0'}{4f_0} - (-)^n [f_0(1+Q_0)]^{1/2} + O\left(\frac{Q_0'}{4}\right). \quad (\text{A17})$$

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An exact solution for a derivative nonlinear Schrödinger equation^{a)}

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A method of solution for the "derivative nonlinear Schrödinger equation"

$$iq_t = -q_{xx} \pm i(q^*q^2)_x$$

is presented. The appropriate inverse scattering problem is solved, and the one-soliton solution is obtained, as well as the infinity of conservation laws. Also, we note that this equation can also possess "algebraic solitons."

By using inverse scattering techniques, we have developed a method for solving the equation

$$iq_t = -q_{xx} \pm i(q^*q^2)_x \quad (1)$$

exactly, which we shall refer to as the "derivative nonlinear Schrödinger equation," or DNLS for brevity.

The DNLS equation has several physical applications, such as the propagation of circular polarized nonlinear Alfvén waves in plasmas¹⁻³ and the propagation of r. f. waves in a plasma.⁴ Exact solitary wave solutions are known^{2,5} as well as the conditions for modulational stability.² Here, we shall only be concerned with the solution when q vanishes as $x \rightarrow \pm\infty$. Solutions where q approaches a nonzero constant as $x \rightarrow \pm\infty$ are also of interest.^{3,5} The inverse scattering for this latter case shall be treated in a later paper.

A very interesting property of the soliton solutions of (1) is that one can have "algebraic" solitons as well as the usual sech, sech^2 , etc. However, these are unstable in the sense that if the initial data is changed by a finite amount, then this soliton will become either (i) radiation and therefore disperse away, or (ii) a very broad sech-like soliton.

First we note that (1) is the integrability condition for

$$v_{1x} + i\xi^2 v_1 = q\xi v_2, \quad (2a)$$

$$v_{2x} - i\xi^2 v_2 = r\xi v_1 \quad (2b)$$

and

$$iv_{1t} = Av_1 + Bv_2, \quad (3a)$$

$$iv_{2t} = Cv_1 - Av_2, \quad (3b)$$

where

$$A = 2\xi^4 + \xi^2 r q, \quad (4a)$$

$$B = 2i\xi^3 q - \xi q_x + i\xi r q^2, \quad (4b)$$

$$C = 2i\xi^3 r + \xi r_x + i\xi r^2 q, \quad (4c)$$

when $r = \pm q^*$. In the usual manner,⁶ we define the Jost

functions by

$$\left. \begin{aligned} \phi &\rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\xi^2 x) \\ \bar{\phi} &\rightarrow \begin{pmatrix} 0 \\ -1 \end{pmatrix} \exp(i\xi^2 x) \end{aligned} \right\} \text{as } x \rightarrow -\infty \quad (5)$$

and

$$\left. \begin{aligned} \psi &\rightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix} \exp(i\xi^2 x) \\ \bar{\psi} &\rightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\xi^2 x) \end{aligned} \right\} \text{as } x \rightarrow +\infty, \quad (6)$$

and the scattering coefficients by

$$\phi = a\bar{\psi} + b\psi, \quad (7a)$$

$$\bar{\phi} = -\bar{a}\psi + \bar{b}\bar{\psi}, \quad (7b)$$

where

$$\bar{a}a + \bar{b}b = 1. \quad (8)$$

We note that, for $r = \pm q^*$,

$$\bar{\phi}(\xi) = \begin{pmatrix} 0 & \pm 1 \\ 1 & 0 \end{pmatrix} \phi^*(\xi^*) \quad (9a)$$

and

$$\bar{\psi}(\xi) = \begin{pmatrix} 0 & 1 \\ \pm 1 & 0 \end{pmatrix} \psi^*(\xi^*) \quad (9b)$$

from whence it follows that

$$\bar{a}(\xi) = a^*(\xi^*), \quad (10a)$$

$$\bar{b}(\xi) = \mp b^*(\xi^*). \quad (10b)$$

The analytical properties of these Jost functions differ only slightly from the Zakharov-Shabat case.⁷ Define

$$\mu^- \equiv \frac{1}{2} \int_{-\infty}^x r q dx \quad (11)$$

and let $\phi_1 = f_1 \exp(i\mu^- - i\xi^2 x)$ and $\xi\phi_2 = [f_2 \exp(-i\mu^-) + \frac{1}{2}iRf_1] \exp(-i\xi^2 x)$, where

$$R = r \exp(i\mu^-), \quad (12a)$$

and also define

$$Q = q \exp(-i\mu^-). \quad (12b)$$

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Then (4) becomes

$$f_{1x} = Q f_2 \exp(-i\mu^-), \quad (13a)$$

$$f_{2x} - 2i\xi^2 f_2 = -\frac{1}{2}iR_x f_1 \exp(i\mu^-). \quad (13b)$$

The reason why we have taken the above decomposition for ϕ_1 and ϕ_2 is simply to obtain Eq. (13) in this form. This is exactly the same form that naturally occurred for the Zakharov-Shabat equation. And thus from those results,⁶ one can immediately know what the analytical properties are. From (13) it can be shown⁶ that if

$$\int_{-\infty}^{\infty} [|Q| + |Q|^2 + |Q_x|] dx < \infty, \quad (14)$$

then $\phi \exp(i\xi^2 x)$, $\psi \exp(-i\xi^2 x)$, and a are analytic functions of ξ for ξ in the upper half ξ^2 plane. As $|\xi| \rightarrow \infty$ for $\text{Im}(\xi^2) > 0$, we have

$$\phi \exp(i\xi^2 x) - \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(i\mu^-) + o(1), \quad (15a)$$

$$\psi \exp(-i\xi^2 x) - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \exp(i\mu^*) + o(1), \quad (15b)$$

and

$$a \rightarrow \exp(i\mu) + o(1), \quad (15c)$$

where

$$\mu^* \equiv \frac{1}{2} \int_x^{\infty} r q dx, \quad (16a)$$

$$\mu \equiv \mu^* + \mu^- \equiv \frac{1}{2} \int_{-\infty}^{\infty} r q dx. \quad (16b)$$

The zeros of a in the upper half ξ^2 plane are the bound state eigenvalues, which we shall designate by ξ_l ($l = 1, 2, \dots, 2N$). If ξ_l is an eigenvalue, then $-\xi_l$ is also an eigenvalue, since a is an even function of ξ . Thus, we will adopt the convention that ξ_{2k} will lie in the first quadrant of the ξ plane, and ξ_{2k+1} will lie in the third quadrant, where $\xi_{2k+1} = -\xi_{2k}$, and $k = 1, 2, \dots, N$. At a zero of a , we have

$$\phi(\xi_l) = b_l \psi(\xi_l). \quad (17)$$

Since b is an odd function of ξ , we shall define $B_k = b_{2k}/\xi_{2k} = b_{2k+1}/\xi_{2k+1}$. From these relations it then follows⁶ (for q on compact support) that

$$\begin{aligned} \bar{\psi}(\xi) \exp(i\xi^2 x) &= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \exp(-i\mu^*) \\ &+ \frac{1}{2\pi i} \int_C \frac{d\xi'}{\xi' - \xi} \frac{b(\xi')}{a(\xi')} \psi(\xi') \exp(i\xi'^2 x), \end{aligned} \quad (18)$$

where the contour C is shown in Fig. 1 and consists of two parts, with ξ and all zeros of a lying between these two parts.

Furthermore, one can give $\psi(\xi)$ by the integral representation

$$\begin{aligned} \psi &= \begin{pmatrix} 0 \\ 1 \end{pmatrix} \exp[i(\xi^2 x + \mu^*)] + \int_x^{\infty} \exp(i\xi^2 s) ds \\ &\times \begin{bmatrix} \xi K_1(x, s) \exp[-i\mu^*(x)] \\ K_2(x, s) \exp[i\mu^*(x)] \end{bmatrix}. \end{aligned} \quad (19)$$

In order for (19) to be valid, it is necessary that

$$\lim_{s \rightarrow \infty} K_1(x, s) = 0, \quad (20a)$$

$$\lim_{s \rightarrow \infty} K_2(x, s) = 0, \quad (20b)$$

$$K_1(x, x) = -\frac{1}{2}q(x) \exp(2i\mu^*) \quad (20c)$$

and for K_1 and K_2 to satisfy

$$(\partial_x - \partial_s)K_1 = qL \exp(2i\mu^*), \quad (21a)$$

$$(\partial_x + \partial_s)L = -\frac{1}{2}iK_1 \exp(-i\mu^*) \partial_x [r \exp(-i\mu^*)], \quad (21b)$$

where

$$L \equiv K_2 - \frac{1}{2}irK_1 \exp(-2i\mu^*). \quad (22)$$

Due to the characteristics in (21), given a q , there exists a solution of (21) which satisfies (20). Thus (19) is valid. Inserting (19) into (18) and using (9b) to determine $\bar{\psi}$, one can obtain, for $y > x$,

$$K_2^*(x, y) - i \int_x^{\infty} K_1(x, s) F'(s+y) ds = 0, \quad (23a)$$

$$\pm K_1(x, y) + F^*(x+y) + \int_x^{\infty} K_2^*(x, s) F^*(s+y) ds = 0, \quad (23b)$$

for $r = \pm q^*$, where

$$F(x) \equiv \frac{1}{2\pi} \int_C \frac{b(\xi)}{a(\xi)} \exp(i\xi^2 z) d\xi, \quad (24a)$$

$$F'(z) \equiv \frac{dF(z)}{dz}. \quad (24b)$$

In deriving (23), we have taken a Fourier transform along the contour R shown in Fig. 1, where

$$\int_R \exp(i\xi^2 L) f(\xi^2) d\xi = 0, \quad (25a)$$

$$\int_R \exp(i\xi^2 L) \xi d\xi = 2\pi\xi(L), \quad (25b)$$

and for $\text{Im}(z^2) > 0$,

$$\int_R \frac{\exp(i\xi^2 L)}{\xi - z} d\xi = 2\pi i \exp(iz^2 L) \theta(L), \quad (25c)$$

$$\int_R \frac{\exp(i\xi^2 L)}{\xi - z} \xi d\xi = 2\pi iz \exp(iz^2 L) \theta(L), \quad (25d)$$

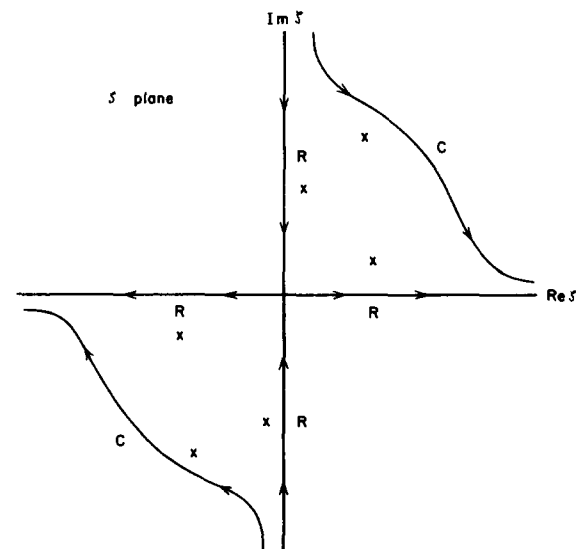


FIG. 1. The contour C and R in the complex λ plane. The crosses indicate where the zeros of a lie.

where $\theta(L)$ is the Heaviside function. Also, since b/a is odd in ξ ,

$$\int_C \frac{b(\xi)}{a(\xi)} \exp(i\xi^2 z) \xi d\xi = 0. \quad (26)$$

One can also simplify (24a) by using $a(-\xi) = a(\xi)$ and $b(-\xi) = -b(\xi)$. Since a is even in ξ , all zeros will occur in pairs. Define $\lambda = \xi^2$ for ξ^2 real and

$$\rho(\lambda) \equiv [b(\xi)/a(\xi)] \xi^{-1}. \quad (27)$$

For the bound states, define $\lambda_k = \xi_{2k}^2 = \xi_{2k+1}^2$, $a'_k = (\partial a / \partial \lambda)|_{\lambda=\lambda_k}$ and $C_k = iB_k/a'_k$. Then one may show that (24a) becomes

$$F(z) = \sum_{k=1}^N C_k \exp(i\lambda_k z) + \frac{1}{2\pi} \int_{-\infty}^{\infty} \rho(\lambda) \exp(i\lambda z) d\lambda, \quad (28)$$

when all of the zeros of a are simple and where N is the total number of distinct values of λ_k .

From (28), we see that the scattering data for this problem is

$$S = \{\rho(\lambda), \lambda \text{ real}; [\lambda_k, C_k]_{k=1}^N\}. \quad (29)$$

Given S , we may construct F as in (27), then one may solve (23) for $K_1(x, y)$, and by (20c), one can obtain $q(x)$ (when $r = \pm q^*$).

The N -soliton solution results upon setting $\rho(\lambda) = 0$. For $N = 1$ and $r = \pm q^*$, letting

$$\lambda_1 = i\Delta^2 \exp[\pm i(\pi/2 - \gamma)] \quad (0 < \gamma < \pi) \quad (29a)$$

$$\eta = \Delta^2 \sin \gamma, \quad (29b)$$

$$\xi = \mp \Delta^2 \cos \gamma, \quad (29c)$$

and

$$C_1 = 2 \frac{\eta}{\Delta} \exp(2i\sigma_0) \exp(2\eta x_0), \quad (30)$$

then one obtains

$$q(x) \exp(2i\mu^*) = \pm 4\Delta \sin \gamma \frac{\exp(2\theta) \exp(-2i\sigma)}{\exp(4\theta) + \exp(\mp i\gamma)}, \quad (31)$$

where

$$\theta \equiv \eta(x - x_0), \quad (32a)$$

$$\sigma \equiv \xi x + \sigma_0. \quad (32b)$$

From (16a) and (31), we have

$$\exp(i\mu^*) = \frac{\exp(4\theta) + \exp(\pm i\gamma)}{\exp(4\theta) + \exp(\mp i\gamma)}, \quad (33a)$$

and thus

$$\mu = \frac{1}{2} \int_{-\infty}^{\infty} r q dx = \pm 2\gamma, \quad (33b)$$

$$q = \pm 4\Delta \sin \gamma \frac{\exp(2\theta) \exp(-2i\sigma)}{\exp(4\theta) + \exp(\pm i\gamma)} \exp(-i\mu^*). \quad (33c)$$

Note that, by (33b), μ is given by the argument of the eigenvalue, λ_1 . For $r = +q^*$, from (29a) and (33b), μ is given by the argument measured from the negative real λ axis, whereas for $r = -q^*$, $-\mu$ is given by the argument measured from the positive, real λ axis.

From (3) and (4), we can obtain the time dependence of the scattering data, which is

$$i\rho_t = -4\lambda^2 \rho \quad (\lambda \text{ real}) \quad (34)$$

and for $k = 1, 2, \dots, N$

$$i\lambda_{kt} = 0, \quad (35a)$$

$$iC_{kt} = -4\lambda_k^2 C_k. \quad (35b)$$

Thus from (29) and (30), we have

$$\sigma_{0t} = 2\Delta^4 \cos 2\gamma, \quad (36a)$$

$$x_{0t} = \pm 4\Delta^2 \cos \gamma. \quad (36b)$$

Algebraic solitons arise whenever $\gamma = \pi$. Letting $\gamma = \pi - \epsilon$ in (29), (32), and (33), and taking the limit of $\epsilon \rightarrow 0$ gives

$$\exp(i\mu^*) = \frac{4\Delta^2(x - x_0) \pm i}{4\Delta^2(x - x_0) \mp i}, \quad (37a)$$

and

$$q = \pm \frac{4\Delta \exp[-2i(\pm \Delta^2 x + \sigma_0)] \exp(-i3\mu^*/2)}{[1 + 16\Delta^4(x - x_0)^2]^{1/2}}. \quad (37b)$$

In the usual manner, one may obtain the infinity of conserved quantities associated with Eqs. (1), (2) and (3). From the analytical properties of $a(\lambda)$, one finds for λ in the upper half λ plane that

$$a(\lambda) = \exp(i\mu) \prod_{k=1}^N \left(\frac{\lambda - \lambda_k}{\lambda - \lambda_k^*} \right) \exp\left(\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\lambda'}{\lambda' - \lambda} \ln \bar{a} a(\lambda') \right). \quad (38)$$

Directly from (12), one may obtain $\ln a(\lambda)$ in an asymptotic series of $1/\lambda$. This is

$$\ln a(\lambda) = i \sum_{n=0}^{\infty} C_n / (2\lambda)^n, \quad (39)$$

where

$$C_0 = \mu \quad (40a)$$

and for $n \geq 1$,

$$C_n = \int_{-\infty}^{\infty} g_n Q \exp(-i\mu^*) dx, \quad (40b)$$

where

$$g_1 = -\frac{1}{2} i \exp(i\mu^*) R_x, \quad (40c)$$

and, for $n > 2$, g_n can be obtained from the recursion relation

$$g_n = -i \partial_x g_{n-1} + Q \exp(-i\mu^*) \sum_{p=1}^{n-2} g_p g_{n-p-1}. \quad (40d)$$

From (38) and (39), one can obtain the C_n 's in terms of the scattering data. For $n \geq 1$, this is

$$C_n = -i \frac{2^n}{n} \sum_{k=1}^N [(\lambda_k^*)^n - (\lambda_k)^n] + \frac{1}{2\pi} \int_{-\infty}^{\infty} (2\lambda)^{n-1} d(2\lambda) \ln \bar{a} a. \quad (41)$$

From (40), the first three C_n 's are

$$C_0 = \int_{-\infty}^{\infty} r q dx, \quad (42a)$$

$$C_1 = -\frac{1}{2} i \int_{-\infty}^{\infty} R_x Q dx, \quad (42b)$$

$$C_2 = \frac{1}{2} \int_{-\infty}^{\infty} [R_x Q_x - i R_x R Q^2] dx, \quad (42c)$$

where R and Q are given by (11).

The conserved quantity C_1 provides the Hamiltonian for the system (1). Let

$$H_1 = 2C_1 = -i \int (qr_x + \frac{1}{2}q^2r^2) dx. \quad (43)$$

Thus $\text{grad}H_1 = (-ir_x + qr^2, iq_x + q^2r)$ and Hamilton's equations are

$$\begin{pmatrix} q_t \\ r_t \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x} \text{grad}H_1 \quad (44)$$

with the symplectic $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \partial/\partial x$. Equation (44) is (1). We introduce the Poisson bracket

$$\langle F, G \rangle = \int_{-\infty}^{\infty} \text{grad}G \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\partial}{\partial x} \text{grad}F dx. \quad (45)$$

If $I[q, r]$ is a functional of q and r and the latter evolves according to (44), then

$$\frac{dI}{dt} = \langle H_1, I \rangle. \quad (46)$$

In particular, if I is any of the conserved quantities K {any of the constants of the motion generated by $\ln[a(x)]$; e.g., the eigenvalues considered as functionals of q and r , or the conserved quantities $\{C_n\}_{n=0}^{\infty}$ }, then $\langle H_1, K \rangle = 0$. All the constants of the motion are in involution and each C_n , $n > 1$, generates a flow for which all the other potential Hamiltonians C_n are conserved. The transformations between the original variables q, r and the scattering data is a canonical one in which the 2-form $\int_{-\infty}^{\infty} \{\delta q \wedge \int^x \delta r + \delta r \wedge \int^x \delta q\} dx$ is preserved. When written in the terms of the scattering data, this expansion will indicate precisely which quantities are to be action and angle variables (they will be proportional to λ_k and $\ln a a^*$ and the arguments of C_k and ρ) but these details have yet to be worked out. Each Hamiltonian is given in terms of the action variables by (41). Note that C_0 is not in the family (41). Indeed matching the

first terms in the asymptotic expansion of (38) gives the identity $C_0 = \frac{1}{2} \int_{-\infty}^{\infty} qr dx = \mu$. The flow generated by C_0 is merely a translation. Note that all the action variables relate to C_n , $n \geq 1$ and thus C_0 can be prescribed independently. This is somewhat similar to the situation for the Korteweg-de Vries equation where the total mass $\int_{-\infty}^{\infty} q dx$ is a constant of the motion not related to the scattering data.

Finally the flow generated by $H_2 = -2C_2$ is

$$\begin{aligned} q_t &= (q_{xx} - 3iqrq_x - \frac{3}{2}q^3r^2)_x, \\ r_t &= (r_{xx} + 3iqr r_x - \frac{3}{2}q^2r^3)_x, \end{aligned} \quad (47)$$

which for $r = \pm iq$ provides yet another integrable model for an integrable system of long lattice waves,

$$q_t = (q_{xx} \pm 3q^2q_x + \frac{3}{2}q^5)_x. \quad (48)$$

Note added in proof: Recently, E. Mjølhus (preprint) has shown that these algebraic solitons occur at the threshold of modulational instability. Also, T. Kawata and H. Inoue (preprint) have solved the inverse scattering problem for Eq. (2) when r and q do not vanish as $x \rightarrow \pm \infty$.

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Absence of ordering in a class of real liquids—Application to nematic liquid crystals

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A classical liquid, the constituents of which are characterized by an internal structure described by a compact connected Lie group, is studied. The order parameter of such systems is shown to vanish for dimension smaller than three. The example of nematic liquid crystals is considered.

1. INTRODUCTION

By now there are several rigorous results on the existence or absence of phase transitions for spin lattice systems.^{1,2} Although the translational symmetry is not an essential ingredient, the lattice, or more precisely the association of the spins with some sites of a given lattice, is an important point of the existing proofs mentioned above. The fact that the spin variables are situated on the sites of a geometrical lattice of E^3 is however, as was already mentioned in Ref. 3, only used to allow an integration on the first Brillouin zone, defined as usual relatively to the given lattice, and consequently to introduce, through the volume elements of this integration, the dimensionality of the system.

The purpose of this note is to show that for the class of systems considered in Ref. 4, that is for a large class of generalized classical spin systems, the argument leading to the absence of ordering, in dimensions one and two, can be worked out without prescribing that the spins be on a lattice, but under the very mild following conditions.

Let R and R' be any arbitrary positions of the constituents of the system (spins or molecules, etc.). We require that, for a given $\gamma > 0$

$$\|R - R'\| \geq \gamma, \quad (1.1)$$

for all pairs R, R' of constituents.

Conditions (1.1) being very weak, it is tempting to consider systems where the positions $\{R\}$ are no longer fixed points of E^3 but dynamical variables satisfying (1.1). In other words, we consider the case of a kind of liquid, the constituents of which are "molecules" having a certain internal structure and interacting with one another in such a way that (1.1) remains valid. Such systems will be appropriate to describe, for example, polar, magnetic molecular systems, or anisotropic molecules such as liquid crystals.

2. FORMALIZATION OF THE PROBLEM

To make things more precise, let us assume we are dealing with a classical system formed of interacting objects contained in a volume $V \subset \mathbb{R}^{\nu}$, ν being the dimension of the space, numbered by the elements of a subset Λ of N . The configuration space Γ is given by

$$\Gamma = \prod_{n \in \Lambda} M_n, \quad (2.1)$$

where each M_n is isomorphic to the vector bundle M of base \mathbb{R}^{ν} and fibers G_{R_n} , $n \in \Lambda$, all G_{R_n} being isomorphic

to a given compact connected Lie group G . In other words, Γ can be looked upon as the usual configuration space for $|\Lambda|$ (equal to the cardinality of Λ) of punctual particles, where each point R_n is replaced by the compact group G_{R_n} . Since we are considering some kind of molecular system, we will assume that the kinetic energy T is a quadratic form in the canonical conjugates of the dynamical matrix. This restriction is not very strong and is satisfied by many physical systems such as molecules performing rigid rotations around their center of mass.

Note added in proof: By this we mean that in the appropriate conjugate coordinates, for which $dq_1 \cdots dq_n$ is a G -invariant measure. T is a quadratic form in the p_i only.

Within this assumption on T , which will be done throughout this paper, the absence of ordering will not depend on T , but only on the interaction part of the potential, to which we now restrict ourselves.

Let $H(\Lambda)$ be the Hamiltonian (interaction part only) of our system,

$$Z(\Lambda) = \int_{\Gamma} \exp[-\beta H(\Lambda)] d\Gamma, \quad (2.2)$$

where $H(\Lambda) \in C^{\infty}(\Gamma; \mathbb{R})$, $d\Gamma$ being the measure on Γ , and $\beta = (k_B T)^{-1}$; then we have for all observables $\phi \in C^{\infty}(\Gamma; \mathbb{C})$, the "thermal average"

$$\langle \phi \rangle_{\Lambda} = Z^{-1}(\Lambda) \int_{\Gamma} d\Gamma(\gamma) \exp[-\beta H(\Lambda)(\gamma)] \phi(\gamma). \quad (2.3)$$

We now specify more precisely the form of the Hamiltonian we want to deal with. We put

$$H(\Lambda) = \sum_{\substack{i, j \in \Lambda \\ i \neq j}} J(R_i - R_j) P(g_i, g_j) + F \sum_{j \in \Lambda} Q(g_j), \quad (2.4)$$

P and Q being uniformly bounded (in g_i, g_j) functions on the compact group $G(\Lambda) = \prod_{i \in \Lambda} G_{R_i}$, with values in \mathbb{R} , F an external (symmetry breaking) coupling field, and J a coupling function satisfying:

1. $J(R) = \infty$ if $\|R\| < \gamma$ (hard core)
2. $\sum_{m=1}^{\infty} |J(R_n - R_m)| (R_n - R_m) \leq W < \infty \forall n$ (2.5)

such that for every configuration R_n the position vectors satisfy, for all p and m , the relations

$$\|R_p - R_m\| \geq \gamma,$$

where W is independent of R_n and of the configuration

$$\{R_m\}_{m=1}^\infty,$$

$$3. J(R) = J(-R).$$

Writing (2.4) in the form $H^0(\Lambda) + FH'(\Lambda)$, we also assume that for all configurations $\{R\}$, compatible with (2.5),

$$H^0(\Lambda)(\{R_i\}; \{g_{R_i} g\}) = H^0(\Lambda)(\{R_i\}; \{g_{R_i}\}) \text{ for all } g \in G. \quad (2.6)$$

At an infinitesimal level, (2.6) implies the relation

$$\sum_{i \in \Lambda} X^{R_i} H^0(\Lambda) = 0, \quad (2.7)$$

for each copy X^{R_i} of any X in the Lie algebra of G .

Our next task is to pass to the thermodynamic limit. For this we note that conditions (2.5) are stronger than the weak tempering condition usually imposed on thermodynamic potentials and that, due to the uniform boundedness of P and Q , Fisher's arguments⁵ can be easily translated to this case, yielding the existence of the thermodynamic stability and of the free energy per particle,

$$f(F) = \lim_{\Lambda \rightarrow \infty} [-(|\Lambda| \beta)^{-1} \times \log \int_{\Gamma} d\Gamma \exp[-\beta H^0(\Lambda) + FH'(\Lambda)]. \quad (2.8)$$

3. BOGOLIUBOV INEQUALITY

We first recall, without proof, the following result of Ref. 4 which is the key of the generalization of classical Bogoliubov inequality. (It may be worthwhile to note that the proof of this lemma does not lean on the existence of a geometrical lattice in L^p .)

Lemma 3.1: Let $(D_\alpha)_{1 \leq \alpha \leq n}$ be a family of differential operators on $G_{\{R\}}(\Lambda)$, for any fixed configuration $\{R\}$, and let $(\phi_\alpha)_{1 \leq \alpha \leq n}$ be a family of functions on $C^\infty(G_{\{R\}}(\Lambda); \mathbb{C})$. Then, for every family $(X_\alpha)_{1 \leq \alpha \leq n}$ of left-invariant complex vector fields on $G_{\{R\}}(\Lambda)$ we have

$$\beta \sum_{\alpha=1}^n \langle \bar{X}_\alpha (X_\alpha H(\Lambda)) \rangle_{\{R\}} \sum_{\gamma=1}^n \langle |D_\gamma \phi_\alpha|^2 \rangle_{\{R\}} \geq \left| \sum_{\alpha=1}^n \langle X_\alpha (D_\alpha \phi_\alpha) \rangle_{\{R\}} \right|^2. \quad (3.1)$$

We now define X_α and D_α in the following way,

$$X_\alpha = \sum_{m \in \Lambda} \exp[i(k, R_m)] X_\alpha^{R_m} \equiv X_\alpha(k), \quad (3.2)$$

$$D_\alpha = \sum_{m \in \Lambda} \exp[-i(k, R_m)] Y_\alpha^{R_m} \equiv Y_\alpha(k),$$

where $(X_\alpha^{R_m})_{1 \leq \alpha \leq n}$ and $(Y_\alpha^{R_m})_{1 \leq \alpha \leq n}$ are two dual bases of the Lie algebra of G_{R_m} which enter the expression of the Casimir operator, and k is an element of \mathbb{R}^p .

Following the lines of Ref. 4 and taking $\phi_\alpha \equiv Q$, we get, by introducing (3.2) into (3.1),

$$\beta \sum_{\gamma} \int_{\tilde{\Delta}} \langle \left| \sum_{m \in \Lambda} \exp[-i(k, R_m)] Y_\gamma^{R_m} Q \right|^2 \rangle_{\{R\}} d^3 k \geq \text{const} |\Lambda|^{-1} |\langle Q \rangle_{\{R\}}|^2 \int_{\tilde{\Delta}} \frac{1}{Ak^2 + FB} d^p k, \quad (3.3)$$

where $\tilde{\Delta}$ is an arbitrary finite region which will be specified later, and A and B are positive constants.

We are now in a position to prove the following theorem.

Theorem 3.1: If

$$\eta = \lim_{F \rightarrow 0} \lim_{\Lambda \rightarrow \infty} Z^{-1}(\Lambda) |\Lambda|^{-1} \int_{\Gamma} Q(g_{\{R_i\}}) \times \exp[-\beta H(\Lambda)(\{R_j\}, \{g_j\})] \prod_{j=1}^{(\Lambda)} dg_{R_j} d^p R_j, \quad (3.4)$$

then $\eta = 0$ for $\nu = 1$ and 2, for $\beta \neq 0$.

Remark: From the assumption made on T it is clear that (3.4) can be defined by including T in the Hamiltonian without changing the result.

Proof: Put $f_\nu(k) = \sum_{m \in \Lambda} \exp[-i(R_m, k)] (Y_j^{R_m} Q)$, for a fixed configuration. Then, since by (2.5), condition (A3) of the Appendix is satisfied, we have, by Theorem A1 that

$$\sum_{m \in \Lambda} |Y_\nu^{R_m} Q|^2 \geq a_\nu(\gamma, \Delta) \int_{\Delta} |f_\nu(k)|^2 d^3 k. \quad (3.5)$$

Interchanging in (3.3) the integration on k with the one giving the thermal average, it can be shown, following the arguments of Ref. 4 that, for $\tilde{\Delta} \equiv \Delta$, (3.3) can be put in the form

$$\beta \sum_{\gamma} \Delta a_\nu(\gamma, \Delta) \sum_{m \in \Lambda} \langle |Y_\nu^{R_m} Q|^2 \rangle_{\{R\}} \geq \text{const} |\Lambda|^{-1} |\langle Q \rangle_{\{R\}}|^2 \times \int_{\Delta} \frac{d^p k}{Ak^2 + FB}. \quad (3.6)$$

It may be worth some value to note the importance of relation (3.6) [or (3.5)]. This importance lies in the fact that, Q being $\{R_m\}$ independent, the lhs of (3.6) is bounded and proportional to $|\Lambda|$ (not to $|\Lambda|^2$).

We also point out that by condition (2.5), A can be chosen $\{R\}$ independent, and thus the integration on the R refers to $Q_{\{R\}}$ only.

Taking these remarks into account, (3.6) can be transformed into the inequality

$$1 \geq |\eta|^2 \mu \beta^{-1} \int_{\Delta} \frac{d^p k}{Ak^2 + FB}, \quad (3.7)$$

where μ is a positive constant and η is given by (3.4). For $\nu = 1$ and 2, this integral is diverging, proving the theorem.

4. THE NEMATIC LIQUID CRYSTAL CASE

In nematic liquid crystals, the long-range orientational order parameter is usually defined by Ref. 6,

$$\eta = \langle P_2(\cos \varphi) \rangle$$

where φ is the angle which the "long" molecular axis makes with a preferred axis and $\langle \cdot \rangle$ is the thermal average. In this definition, due to Tsvetkov,⁷ the molecules are assumed to be cylindrically symmetric and η takes into account the fact that the preferred axis is neither polar nor ferroelectric.

The order parameter so defined describes very satisfactorily the degree of alignment of the molecules. It is

moreover coupled, in a very simple way to many physical quantities (see Ref. 6), and enters the main statistical models which attempt to describe the behavior of nematic liquid crystals, which all are, in some way, generalizations of the Maier and Saupe model.⁸ In this last one, the stability of the nematic phase is assumed to come from the dipole-dipole part of the anisotropic dispersion forces and the transition point calculated through the mean field approximation method. In all the improved version of this theory the main changes consist, on the one hand, in choosing an improve mean field potential, with terms proportional to $P_2(\cos\varphi)$ and $P_4(\cos\varphi)$ and, on the other hand, in taking into account the short-range order interactions which remain very strong in the neighborhood of the transition point but are ruled out by the mean field method. Finally, a possible polar contribution may be present, leading in addition to a term proportional to $P_1(\cos\varphi)$. (P_1, P_2 , and P_4 are here Legendre polynomials.)

It should be remarked that if the model is not treated within the mean field approximation the short- and long-range order interactions are functions of the angles between the different pairs of molecular axes (and not of the angles between these axes and a preferred direction), leading to assume, for the interaction Hamiltonian, the form

$$H(\Lambda) = \sum_{n,m \in \Lambda} \sum_r J_r(R_n - R_m) P_r(\cos\varphi_{n,m}), \quad (4.1)$$

where the P_r are Legendre polynomials, $\varphi_{n,m}$ is the angle between the axis of the molecules n and m , and the sum on n runs over a finite number of terms.

Our purpose now is to see that for a system governed by the Hamilton (4.1), Theorem (3.1) holds. To do this, we note that these molecules cannot, being relatively thick, penetrate each other; moreover, since the intermolecular forces are decreasing rapidly (Van der Waals type) conditions (2.5) are valid for each J_r . It is important to note here that we assume that conditions (2.5) are valid due to a kind of screening leading to a Van der Waal type interaction. The argument would however not apply for a strictly dipole-dipole interaction. The only requirement which remains for the fulfillment of Theorem (3.1), is condition (2.6). To show that (2.6) is valid, we note that if \mathbf{u} is any fixed vector of E^3 , $\cos\varphi_{ij} = (g_i\mathbf{u}, g_j\mathbf{u})$, where g_i and g_j are rotations which send \mathbf{u} into the direction of the principal axes of the molecules i and j , respectively. It is then easy to see that (2.6) is satisfied and consequently that the Hamiltonian (4.1) leads to a system for which $\eta=0$, for dimensions one and two.

It would be hazardous however to conclude that two-dimensional liquid crystals do not exhibit phase transitions, for the model used is too simple to account rigorously for all the detailed interactions of such systems.

In fact, it neglects the following important facts:

1. some possible anisotropy in the interaction not included into (4.1) which does not satisfy (2.6),
2. the effect of volume of the molecules (hard rods liquid) which cannot penetrate each other and can lead, for high density to a phase transition,⁶

3. the possibility that the interaction between molecules does not satisfy conditions (2.5), i. e., is relatively long range.

CONCLUSIONS

We have shown that in the classical case, the Mermin-Wagner argument, properly generalized to a larger class of systems, remains valid even if the underlying lattice to which the constituents of the system are generally bound is removed. This is the case for nematic liquid crystals which are analyzed in the second part of this paper.

It would be interesting to see if the importance attached to this lattice can also be weakened in the proof of existence of phase transitions.²

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APPENDIX

Making use of methods similar to those introduced by Ingham,⁹ we prove the following theorem.

Theorem (A.1): Let

$$f(q) = \sum_{n \in \Lambda \subset \mathbb{Z}} a_n \exp[i(\lambda_n, q)], \quad q_1, \lambda_n \in \mathbb{R}^\nu, \quad (A1)$$

where the elements of the set $\{\lambda_n\}_{n \in \Lambda}$ satisfy

$$\|\lambda_n - \lambda_m\| \geq \gamma > 0 \text{ for all } m \neq n. \quad (A2)$$

We then have, for $\nu=1, 2, \dots$,

$$\sum_{n \in \Lambda} |a_n|^2 \geq a_\nu(\gamma, \Delta) \int_\Delta |f(q)|^2 d^\nu q, \quad (A3)$$

where Δ is an arbitrary closed sphere centered at $q=0$ and $a_\nu(\gamma, \Delta)$ is strictly positive for $\gamma > 0$, independent of Λ . (This choice of Δ is done for convenience only, it can be generalized to other closed sets.)

Proof: Let $k(q)$ be a continuous absolutely integrable function on \mathbb{R}^ν satisfying

$$k(q) \geq 0, \quad k(q) = k(\|q\|), \quad \text{and } k(q) \neq 0 \text{ in } \Delta. \quad (A4)$$

With (A1) we have

$$\int_{\mathbb{R}^\nu} k(q) |f(q)|^2 d^\nu q = \sum_{m,n \in \Lambda} a_m \bar{a}_n K(\lambda_m - \lambda_n), \quad (A5)$$

where

$$K(u) = \int_{\mathbb{R}^\nu} k(q) \exp[i(q, u)] d^\nu q. \quad (A6)$$

Using (A4) and the fact that $2|a_n a_m| \leq |a_n|^2 + |a_m|^2$, we get

$$\begin{aligned} \int_{\mathbb{R}^\nu} k(q) |f(q)|^2 d^\nu q \\ \leq \sum_{n \in \Lambda} |a_n|^2 \{K(0) + \sum_{\substack{m \in \Lambda \\ m \neq n}} |K(\lambda_m - \lambda_n)|\}. \end{aligned}$$

Let $M^{-1} = \inf_{q \in \Lambda} k(q)$. By (A4), M is different from zero, and we can write the following inequalities:

$$\begin{aligned} \int_\Delta |f(q)|^2 d^\nu q \leq M \int_\Delta k(q) |f(q)|^2 d^\nu q \leq M \int_{\mathbb{R}^\nu} k(q) |f(q)|^2 d^\nu q \\ \leq M \sum_{n \in \Lambda} |a_n|^2 \{K(0) + \max_{\substack{n \in \Lambda \\ n \neq m}} \sum_{m \in \Lambda} |K(\lambda_m - \lambda_n)|\}. \end{aligned} \quad (A7)$$

For $\nu=1$ Ingham⁹ has shown that (A7) is, for $\Lambda \rightarrow \infty$, a converging series for the following choices of $k(q)$ and Δ :

$$k(q) = \begin{cases} \cos(\pi/2T)q, & |q| \leq T, \\ 0 & |q| > T, \end{cases}$$

and $\Delta = [-T/2, T/2]$. For $\nu > 1$ we take

$$k(q) = \exp[-(1 + \|q\|^2)^{1/2}]/(1 + \|q\|^2)^{1/2}. \quad (\text{A8})$$

Introducing the spherical coordinates $\|q\| = r$, $= r, \theta_1, \dots, \theta_{\nu-1}$, where $0 \leq r < \infty$, $0 \leq \theta_1 \leq 2\pi$, $0 \leq \theta_k < \pi$ for $k \neq 1$ and taking into account for the symmetry of $k(r)$, we have

$$\begin{aligned} K(u) &= \int_0^\infty dr \int_0^\pi d\theta_{\nu-1} \cdots \int_0^\pi d\theta_1 \frac{\Gamma(\nu/2)}{\pi^{\nu/2}} r^{\nu-1} \\ &\quad \times \sin^{\nu-2}\theta_{\nu-1} \cdots \sin\theta_2 k(r) \exp(ir\|u\| \cos\theta_{\nu-1}) \\ &= \frac{\Gamma(\nu/2)}{\Gamma((\nu-1)/2)\sqrt{\pi}} \int_0^\infty dr r^{\nu-1} k(r) \int_1^1 dx (1-x^2)^{(\nu/2-1)-1/2} \\ &\quad \times \exp(ir\|u\|x). \end{aligned}$$

But we have (see for example Ref. 10, p. 553)

$$\int_{-1}^1 \exp(ixt) (1-t^2)^{(n-1)/2} dt = \frac{\sqrt{\pi} \Gamma((n+1)/2) J_{n/2}(x)}{(x/2)^{n/2}}$$

so that

$$K(u) = \frac{\Gamma(\nu/2) 2^{\nu/2-1}}{\|u\|^{\nu/2-1}} \int_0^\infty dr r^{\nu/2} k(r) J_{\nu/2-1}(r\|u\|).$$

This Hankel transformation can be performed (see Ref. 11, p. 31), yielding

$$K(u) = \Gamma(\nu/2) 2^{\nu/2-1} \left(\frac{2}{\pi}\right)^{1/2} \frac{K_{(\nu-1)/2}[(1 + \|u\|^2)^{1/2}]}{(1 + \|u\|^2)^{(\nu-1)/4}}, \quad (\text{A9})$$

where the $K_{(\nu-1)/2}$ are modified Bessel functions (see, for example, Refs. 12 and 13).

For integer or half-integer index, the modified Bessel functions are monotone decreasing and fall off exponentially for large values of their arguments.

$K(0)$ being finite, our next task is to show that $\alpha_\nu(\gamma, \Delta)$ is Λ independent. We do this by showing that the rhs of (A7) is a convergent series, for Λ going to infinity, and bounded by a quantity independent of the configuration Λ .

We note that, $K(u)$ being monotone decreasing, the rhs of (A7) will attain its maximum value for a configuration in which the points λ_m are, within conditions (A2), as close as possible to one another. This can be achieved by considering the λ_m as centers of balls of radius $\gamma/2$ forming a close-packed set.

We define in this set a family of spheres centered at λ_n and having radius $\gamma, 2\gamma, 3\gamma, \dots$. The number of balls having their centers between the spheres of radius $(P-1)\gamma$ and $P\gamma$ is certainly smaller than the number N_{P-1} of balls contained in the one of radius $(P+1)\gamma$. But N_{P-1} is itself smaller than the ratio of the volume of the sphere of radius $(P+1)\gamma$ over the one of a ball, that is, $N_{P-1} < (P+1)^\nu 2^\nu$.

With this bound we have, using the monotonicity of $K(u)$, that

$$\begin{aligned} &\sum_{m \in Z^\nu} |K(\lambda_m - \lambda_n)| \\ &\leq \frac{\Gamma(\nu/2)}{\sqrt{\pi} 2^{(\nu+1)/2}} \sum_{P=1}^\infty (q+1)^\nu \frac{K_{(\nu-1)/2}[(1 + (P-1)^2 \gamma^2)^{1/2}]}{[1 + (P-1)^2 \gamma^2]^{(\nu-1)/4}} \end{aligned}$$

is a convergent series which yields the required bound, and proves the theorem.

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Time-dependent scattering theory for infinite delta function potentials in one dimension

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Existence of the Møller wave operators is proved for a system of n quantum mechanical particles interacting through infinite delta function potentials in one dimension.

INTRODUCTION

There has been some discussion in the literature of n -body quantum-mechanical systems in one dimension with interaction between the particles provided by "infinite delta function potentials" (see for example, Refs. 1, 2). Such systems have extremely simple properties and are worth study for this very reason. Scattering theory for these systems (and others) has been analyzed in using time-independent methods. The purpose of the present note is merely to point out that the corresponding time-dependent version of scattering theory can be given for these systems: the Møller wave operators exist and the S matrix is unitary. The proofs are very simple, and in the present author's opinion some salient features of the theory stand out more clearly in the time-dependent version.

1. THE HAMILTONIAN

To reinforce the reader's intuition, we consider first the case of one particle in a potential. We wish to make sense of the operator

$$H = -\frac{1}{2m} \frac{d^2}{dx^2} + \infty \delta(x) \quad (1)$$

on the Hilbert space $L^2(\mathbf{R})$. Intuitively, the idea to be exploited is that the particle cannot pass through the origin. Thus it is natural to view $L^2(\mathbf{R})$ as the direct sum of $L^2(-\infty, 0)$ and $L^2(0, \infty)$. On each of the latter spaces, H should act like the free Hamiltonian $H_0 = -(1/2m)d^2/dx^2$ with zero boundary conditions at $x=0$. To apply this latter operator to a function $\psi \in L^2(0, \infty)$ means: Take the Fourier sine transform $\hat{\psi}$ of ψ , multiply $\hat{\psi}$ by $k^2/2m$, and take the inverse Fourier sine transform of the result. This is equivalent to the following: Take the odd extension of ψ to obtain a function ψ_{odd} in $L^2(\mathbf{R})$, apply the free Hamiltonian H_0 [considered as an operator on $L^2(\mathbf{R})$ in the usual way] to ψ_{odd} , and truncate $H_0\psi_{\text{odd}}$ to obtain a function in $L^2(0, \infty)$. By this kind of analysis, we arrive at the following description of the operator H : Define operators P_{\pm} and A on $L^2(\mathbf{R})$ as follows:

$$(P_+\psi)(x) = \begin{cases} \psi(x) & (x > 0), \\ 0 & (x < 0), \end{cases} \quad (2)$$

$$(P_-\psi)(x) = \begin{cases} 0 & (x > 0), \\ \psi(x) & (x < 0), \end{cases} \quad (3)$$

$$(A\psi)(x) = \psi(x) - \psi(-x). \quad (4)$$

Then

$$H = P_+H_0P_+ + P_-H_0P_- \quad (5)$$

Naturally the situation we have just discussed is equivalent to a two-body problem in which the center-of-mass coordinate has been separated out. If we interpret x as the relative coordinate $x_1 - x_2$ of this two-body problem, then the conditions $x > 0$ and $x < 0$ correspond to $x_1 > x_2$ and $x_2 > x_1$. The definition of the n -body Hamiltonian

$$H = \sum_{i=1}^n -\frac{1}{2m_i} \frac{d^2}{dx_i^2} + \sum_{i < j} \infty \delta(x_i - x_j) \quad (6)$$

is given in terms of operators projecting on subspaces of $L^2(\mathbf{R}^n)$ in which a certain order $x_{i_1} > x_{i_2} > \dots > x_{i_n}$ prevails among the particle coordinates.

Let S_n be the symmetric group on n elements, and for each $\pi \in S_n$ let S_π be the following subset of \mathbf{R}^n :

$$S_\pi = \{(x_1, \dots, x_n) \mid x_{\pi 1} > x_{\pi 2} > \dots > x_{\pi n}\}. \quad (7)$$

Let P_π be the following projection in $L^2(\mathbf{R}^n)$:

$$(P_\pi\psi)(x_1, \dots, x_n) = \begin{cases} \psi(x_1, \dots, x_n) & \text{if } (x_1, \dots, x_n) \in S_\pi, \\ 0 & \text{otherwise.} \end{cases} \quad (8)$$

Let $\sigma(\pi)$ be the parity of the permutation π , and let A be the following operator on $L^2(\mathbf{R}^n)$:

$$(A\psi)(x_1, \dots, x_n) = \sum_{\pi \in S_n} \sigma(\pi) \psi(x_{\pi 1}, x_{\pi 2}, \dots, x_{\pi n}). \quad (9)$$

It is easy to verify that

$$P_\pi A P_\pi = P_\pi, \quad A P_\pi A = A. \quad (10)$$

Writing

$$H_0 = \sum_{i=1}^n -\frac{1}{2m_i} \frac{d^2}{dx_i^2}, \quad (11)$$

the definition of H is now simply

$$H = \sum_{\pi \in S_n} P_\pi H_0 P_\pi. \quad (12)$$

We have correspondingly

$$e^{iHt} = \sum_{\pi \in S_n} P_\pi \exp(iH_0 t) A P_\pi. \quad (13)$$

It should be noted that H and H_0 both commute with A .

2. SCATTERING THEORY

We will establish existence of the Møller wave operators

$$W_{\pm} = s\text{-}\lim_{t \rightarrow \pm\infty} \exp(iHt) \exp(-iH_0t). \quad (14)$$

We do not attempt the usual proof in which $\exp(iHt) \times \exp(-iH_0t)$ is differentiated with respect to t , because H and H_0 do not have the same domain. Instead we proceed as follows: Let $F: L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ denote the operation of Fourier transformation in all the variables. Let C_t be the operator defined for $t \neq 0$ by

$$(C_t\psi)(x_1, \dots, x_n) = \frac{(m_1 \dots m_n)^{1/2}}{(it)^{n/2}} \exp\left(i \sum_{i=1}^n \frac{m_i x_i^2}{2t}\right) \times (F\psi)\left(\frac{m_1 x_1}{t}, \dots, \frac{m_n x_n}{t}\right). \quad (15)$$

Then we have for any $\psi \in L^2(\mathbb{R}^n)$ (see Ref. 3)

$$\lim_{t \rightarrow \pm\infty} \|\exp(-iH_0t)\psi - C_t\psi\| = 0. \quad (16)$$

Now

$$\begin{aligned} \exp(iHt) \exp(-iH_0t) &= \sum_{\mathbf{r} \in S_n} P_{\mathbf{r}} A \exp(iH_0t) P_{\mathbf{r}} \exp(-iH_0t) \\ &= \sum_{\mathbf{r} \in S_n} P_{\mathbf{r}} A B_{\mathbf{r}}(t), \end{aligned} \quad (17)$$

where

$$B_{\mathbf{r}}(t) = \exp(iH_0t) P_{\mathbf{r}} \exp(-iH_0t). \quad (18)$$

Let $\varphi, \psi \in L^2(\mathbb{R}^n)$. By (16) we have (in the sense that the difference of the two sides goes to zero)

$$\begin{aligned} (\varphi, B_{\mathbf{r}}(t)\psi) &= (\exp(-iH_0t)\varphi, P_{\mathbf{r}} \exp(-iH_0t)\psi) \xrightarrow{t \rightarrow \pm\infty} (C_t\varphi, P_{\mathbf{r}} C_t\psi) \\ &= (m_1 \dots m_n / |t|^n) \int_{\mathbb{R}^n} (F\varphi)(m_1 x_1/t, \dots, m_n x_n/t) \\ &\quad \times P_{\mathbf{r}}(F\psi)(m_1 x_1/t, \dots, m_n x_n/t) dx_1 \dots dx_n. \end{aligned} \quad (19)$$

Making the change of variables $k_1 = m_1 x_1/t, \dots, k_n = m_n x_n/t$, we obtain

$$\begin{aligned} (\varphi, B_{\mathbf{r}}(t)\psi) &\xrightarrow{t \rightarrow \pm\infty} \int \overline{(F\varphi)(k_1, \dots, k_n)} P_{\mathbf{r}} \\ &\quad \times (F\psi)(k_1, \dots, k_n) dk_1 \dots dk_n, \end{aligned} \quad (20)$$

where $+\pi = \pi$ and $-\pi$ is defined as follows: If

$$\pi = \begin{pmatrix} 1 & 2 & \dots & n \\ \pi 1 & \pi 2 & \dots & \pi n \end{pmatrix},$$

then

$$-\pi = \begin{pmatrix} 1 & 2 & \dots & n \\ \pi n & \pi(n-1) & \dots & \pi 1 \end{pmatrix}.$$

Equation (20) can be rewritten as follows:

$$B_{\mathbf{r}}(t) \xrightarrow{t \rightarrow \pm\infty} F^{-1} P_{\mathbf{r}} F. \quad (21)$$

Thus

$$\exp(iHt) \exp(-iH_0t) \xrightarrow{t \rightarrow \pm\infty} \sum_{\mathbf{r} \in S_n} P_{\mathbf{r}} A F^{-1} P_{\mathbf{r}} F \equiv W_{\pm}. \quad (22)$$

Now using (10) and the facts that $F^* = F^{-1}$ and F commutes with A , we have

$$\begin{aligned} W_{\pm}^* W_{\pm} &= \sum_{\mathbf{r}, \mathbf{r}' \in S_n} F^{-1} P_{\mathbf{r}'} F A P_{\mathbf{r}} P_{\mathbf{r}'} A F^{-1} P_{\mathbf{r}} F \\ &= \sum_{\mathbf{r} \in S_n} F^{-1} P_{\mathbf{r}} F A P_{\mathbf{r}} A F^{-1} P_{\mathbf{r}} F \\ &= \sum_{\mathbf{r} \in S_n} F^{-1} P_{\mathbf{r}} F A F A F^{-1} P_{\mathbf{r}} F \\ &= \sum_{\mathbf{r} \in S_n} F^{-1} P_{\mathbf{r}} F = I. \end{aligned} \quad (23)$$

Since the unitary operator $\exp(iHt) \exp(-iH_0t)$ converges weakly to W_{\pm} , and since by (23) W_{\pm} is an isometry, it follows that the convergence in (22) is in fact strong. Thus existence of a scattering theory in the time-dependent sense is established. A calculation similar to (23) shows that $W_{+}^* W_{-}^* = I$ so that, as expected in a theory with no bound states, the Møller wave operators are unitary. The S matrix $W_{+}^* W_{-}$ is then obviously unitary. A calculation similar to (23) yields

$$\begin{aligned} S = W_{+}^* W_{-} &= \sum_{\mathbf{r} \in S_n} F^{-1} P_{\mathbf{r}} A P_{-\mathbf{r}} F \\ &= \sum_{\mathbf{r} \in S_n} F^{-1} P_{-\mathbf{r}} A P_{\mathbf{r}} F. \end{aligned} \quad (24)$$

Viewed in momentum space, the S matrix has the extremely simple form

$$F S F^{-1} = \sum_{\mathbf{r} \in S_n} P_{-\mathbf{r}} A P_{\mathbf{r}}. \quad (25)$$

This equation states that a contribution to the incoming wave function at given momenta $k_{\mathbf{r}1} > k_{\mathbf{r}2} > \dots > k_{\mathbf{r}n}$ (particle πi having momentum $k_{\mathbf{r}i}$ will produce a contribution to the outgoing wave function in which particle $\pi 1$ has momentum $k_{\mathbf{r}n}$, particle $\pi 2$ has a momentum $k_{\mathbf{r}(n-1)}$, etc. This is the expected result: The scattering at given $k_{\mathbf{r}1} > k_{\mathbf{r}2} > \dots > k_{\mathbf{r}n}$ exactly mimics the behavior of classical point particles on a line undergoing elastic collisions, in which they exchange momenta.

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A theory of the electromagnetic two-body interaction

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A theory of the electromagnetic two-body interaction is described which leads to equations of motion solvable by local (numerical) integration.

1. INTRODUCTION

Although Newton's action-at-a-distance theory of gravity is similar to Coulomb's Law for charged particles, it was found that its structure is inadequate to describe completely the electromagnetic force because it assumes "instantaneous" interaction. The effort to overcome this inadequacy lead to Maxwell's equations which, while adequate for practical applications, are, at the most basic level, beset with an impediment—that they do not lead to a closed set of coupled equations of motion for two or more charged point particles. Instead one particle is first considered as a current for which Maxwell's equations are solved for the values of the field variables at the location of the second particle whose response is determined by the Lorentz force law. Then, the second particle is considered as a current whose fields perturb the motion of the first current. The recalculated first current is then used to compute more accurate values of the field variables, etc. This is continued back and forth to obtain the solutions to the desired degree of accuracy.

Reacting to this situation, Fokker developed a closed formulation for the electromagnetic force by incorporating light-cone interaction into the action-at-a-distance mechanics.¹ Essentially he found a Lagrangian which is not merely the sum of individual Lagrangians whose variation yields coupled equations of motion. This Lagrangian, however, produced yet another complexity: It led to simultaneous advanced and retarded interaction for each particle. This feature is problematic on two levels. First, it raises questions of causality because it would mean that the present is always partially conditioned by all of the future, contrary to observation. Secondly, it introduces the calculational complication of precluding the known methods of integrating the equations of motion (this point will be discussed below).

No resolutions for the causality difficulties of the *pure* two-particle problem appear to have been proposed; in fact, apparently the only attempt at resolution immerses the problem in a many body universe by invoking radiation absorbers at infinity.² Moreover, although integration of the pure two-particle equations has been attempted, thus far the proposed schemes are clearly only approximation techniques or useful in severely restricted circumstances.^{3,4}

This problem continues to be of great interest and is being studied from many perspectives. Some of these can be found in Refs. 5–9.

It is the purpose of this article to describe a theoretical formulation of the electromagnetic force whose equations of motion can be integrated by known methods and in which advanced interaction, although not completely eliminated, appears at most as an effect of only limited extent. The essence of this formulation, first presented using Cartan's principle and modern differential geometry,¹⁰ will be elaborated herein avoiding abstruse techniques.

2. THE THEORY

The essence of this theory is that it has a single independent parameter which is given no *a priori* physical role (although it has a *posteriori* physical utility); its function is analogous to that of a step counter in a numerical calculation. It does have *a priori* mathematical significance, however, as a dynamical parameter in the sense that it is the independent variable for which the canonical variables are dependent. The only objects with physical significance in this formulation are the world lines; everything else, including the independent parameter, is a mathematical aid to their calculation.

Let \mathbf{x}_j be the Minkowski configuration four-vector with components x_j, y_j, z_j, ict_j of the j th particle. Let $d\mathbf{x}_j$ be a differential displacement along the j th particle's orbit. Two such differentials tangent to arbitrary points p and p' on orbits j and k are related to each other by the Lorentz transformation, $L(p, p', j, k)$, between the instantaneous rest frames of j and k at p and p' ; i. e., given $d\mathbf{x}_j|_p, d\mathbf{x}_k|_{p'}$, is essentially defined by

$$d\mathbf{x}_k|_{p'} = L(p, p', j, k) d\mathbf{x}_j|_p. \quad (2.1)$$

Thus, the differential of arc length, $(d\mathbf{x} \cdot d\mathbf{x})^{1/2}$, is invariant because at any point p' it satisfies

$$\begin{aligned} (d\mathbf{x}_k|_{p'} \cdot d\mathbf{x}_k|_{p'})^{1/2} &= (d\mathbf{x}_j|_p L^* \cdot L d\mathbf{x}_j|_p)^{1/2} \\ &= (d\mathbf{x}_j \cdot d\mathbf{x}_j)^{1/2}. \end{aligned} \quad (2.2)$$

All such differentials may, therefore, be set equal to the common differential $c d\tau$, where c is the speed of light and τ is the independent parameter which assumes the units of time; i. e.,

$$c d\tau = (d\mathbf{x}_j \cdot d\mathbf{x}_j)^{1/2} = (d\mathbf{x}_k \cdot d\mathbf{x}_k)^{1/2}. \quad (2.3)$$

Dividing (2.3) by c and rewriting yields

$$d\tau = dt_j \gamma_j^{-1} = dt_k \gamma_k^{-1}, \quad (2.4)$$

where $\gamma_j^{-1} \triangleq [1 - (\mathbf{v}_j/c)^2]^{1/2}$ in the customary notation.

Digressing momentarily, observe that a particle's proper time, $\Delta\tau_j$, in this formulation is computed by integration from (2.4) to be

$$\Delta\tau_j = \int_{\Delta t_j} \gamma_j dt_j. \quad (2.5)$$

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Because the γ_j are not in general equal, it follows that the values of $\Delta\tau_j$ for different particles are also, in general, unequal. Although a single variable is the proper time for each particle, its values are not simultaneously (i. e., for equal $t_0 + \Delta t_j$) relevant to each particle.

Continuing, let four-velocities be defined as

$$\mathbf{v}_j \triangleq d\mathbf{x}_j/d\tau \equiv \gamma_j(\mathbf{v}_j, ic) \equiv \dot{\mathbf{x}}_j \quad (2.6)$$

and momenta as $m_j\mathbf{v}_j$, where m_j is the j th particle's rest mass. With these definitions, the four-vector version of Hamilton's principle

$$\delta \int_{\tau_1}^{\tau_2} \mathcal{L}(\mathbf{x}_j, \mathbf{v}_j, \tau) d\tau = 0, \quad (2.7)$$

where [for N (number of particles) = 2]

$$\begin{aligned} \mathcal{L} = & \sum_{j=1}^2 [m_j(\mathbf{v}_j \cdot \mathbf{v}_j)^{1/2} \\ & - 2 \sum_{k \neq j}^2 e_j e_k \int_{-\infty}^{\tau} \mathbf{v}_j(\tau) \cdot \mathbf{v}_k(\tau') \delta((\mathbf{x}_j(\tau) - \mathbf{x}_k(\tau'))^2) d\tau'], \end{aligned} \quad (2.8)$$

yields equations of motion coupled by only two interactions. (Because of the upper limit on the integral, not all possible interactions are included.)

There are, however, two forms these equations can take, depending on the character of $\mathbf{x}_j(\tau) - \mathbf{x}_k(\tau)$ for a particular value of τ ; case I, when it is spacelike

$$m_j(\ddot{\mathbf{x}}_j)^\mu = (e_j/c) \left(\sum_{k \neq j}^2 F_k \Big|_{\text{ret}} \right)^{\mu\nu} (\dot{\mathbf{x}}_j)_\nu, \quad j=1,2, \quad (2.9)$$

and case II when it is time-like ($t_b - t_a > 0$)

$$m_a(\ddot{\mathbf{x}})^\mu = (e_a/c) (F_b \Big|_{\text{ret}} + F_b \Big|_{\text{adv}})^{\mu\nu} (\dot{\mathbf{x}}_a)_\nu, \quad m_b \ddot{\mathbf{x}}_b = 0, \quad (2.10)$$

where

$$F_k^{\mu\nu} = 2e_k \int_{-\infty}^{\tau} (\dot{\mathbf{x}}_k^\nu \partial_\mu - \dot{\mathbf{x}}_k^\mu \partial_\nu) \delta((\mathbf{x}_j(\tau) - \mathbf{x}_k(\tau'))^2) d\tau'. \quad (2.11)$$

(For $N > 2$, complex combinations of (2.9) and (2.10) may hold.)

Case I appears to be more natural, each particle proceeds under the retarded influence of the other. Case II is entirely novel; here one particle (b say) has punctured the future light cone of the other (a) so that the further motion of b is unaffected by a which responds, however, to both retarded and advanced signals from b .

An interesting possibility is that a system might switch back and forth between cases I and II. Consider, for example, two oppositely charged particles, one very massive, the other not. Suppose they are initially constrained such that both their world lines are pure timelike up to a time t_0 when they are released. At this point the lighter particle would accelerate towards its partner, which, by comparison, would remain virtually stationary. The extension of these world lines into the future beyond t_0 can be computed according to (2.9). The world line of the massive particle on a Minkowski diagram would continue virtually parallel to the segment preceding t_0 , and filar marks corresponding to increments of τ would be evenly spaced. The

world line of the lighter particle would both curve and be extended by increasingly longer increments for each incremental increase of τ . Because it is asymptotically approaching lightlike line, where an infinitely long line on the diagram has zero length, filar marks on the light particle's world line appear to be at increasing intervals. This disparity will cause the lighter particle at some point to puncture the future light cone of the heavy partner and the system will pass into the case II regime where the lighter particle is free and its world line straight. It can be shown that eventually the lighter particle will re-emerge and the system again enter the case I regime.

3. COMPARISON WITH FOKKER'S FORMULATION

The features peculiar to this theory can best be delineated by comparison with Fokker's formulation.¹ The most outstanding difference is that Fokker's formulation does not exploit (2.3) and therefore employs a separate independent parameter for each particle. Fokker's Lagrangian is not simply the sum of individual Lagrangians patched together in an *ad hoc* manner; he argued that a truly fundamental formulation should proceed from the variation of a *single* system Lagrangian to a set of coupled equations of motion. The Lagrangian \mathcal{L}_F ,

$$\begin{aligned} \mathcal{L}_F = & \sum_j^N L_j = \sum_j^N \left(m_j(\mathbf{v}_j \cdot \mathbf{v}_j)^{1/2} \right. \\ & \left. - \sum_{k \neq j}^N e_j e_k \int_{-\infty}^{\tau} \mathbf{v}_j(\tau_j) \cdot \mathbf{v}_k(\tau_k) \delta((\mathbf{x}_j(\tau_j) - \mathbf{x}_k(\tau_k))^2) d\tau_k \right), \end{aligned} \quad (3.1)$$

satisfies these criteria and leads, by means of the variation

$$\delta \int \sum_j^N L_j d\tau_j, \quad j=1,2,\dots,N, \quad (3.2)$$

to the equations of motion

$$m_j(\ddot{\mathbf{x}}_j(\tau_j))^\mu = \frac{e_j}{2c} \sum_{k \neq j}^N (F \Big|_{\text{adv}} + F \Big|_{\text{ret}})_{k\nu}^{\mu\nu} (\dot{\mathbf{x}}_j(\tau_j))_\nu, \quad j=1,2,\dots,N. \quad (3.3)$$

These equations, however, cannot be integrated by a local procedure as is obvious if one imagines attempting a machine integration of the i th equation at a given value of τ_i . Such an integration; i. e., a calculation of an incremental extension of the worldline for an incremental increase in τ_i , requires knowledge of the j th world line on the forward light cone of the i th particle, which, in order to be computed, requires knowledge of the i th world line on the forward light cone of the j th particle, but this portion of the orbit is yet to be computed, etc., *ad infinitum*. In effect, the solution is needed as initial data in order to compute the solution in this way.

Of course, advanced interaction could be precluded by changing the upper limit of integration in (3.1) to τ_{ij} , where τ_{ij} is that value of τ_i which includes only the retarded potential from the j th particle; however, as τ_{ji} would then also be in (3.1), it could be written as the sum of individual Lagrangians and therefore would not qualify as a system Lagrangian.

Schemes can be imagined which circumvent this problem by some sort of global approach; i. e., by seeking

the whole solution at once. For example, perhaps the solution could be found as the limit of a technique each successive step of which gave a closer approximation to the entire world line. At present, however, such techniques appear not to have been developed—Eqs. (3.3) are in general numerically and analytically unsolvable.

Equations (2.9) and (2.10), on the other hand, can always be integrated by machine because the information needed to compute each incremental increase of any world line in both cases I and II has already been computed. Also by imagining a machine calculation, it is clear that if each particle's world line between the past and future with respect to the same but otherwise arbitrary light cone is given as initial data, then the system of world lines can be extended by calculation indefinitely into the future or the past. Although this type and amount of initial data is greater than the customary Cauchy data $[x(\tau_0), \dot{x}(\tau_0)]$, it is a general characteristic of differential-delay equations that Cauchy data are insufficient to determine a particular solution as enough initial data must be given to span the delay.^{11,12}

4. RADIATION REACTION

Because the classical derivation of the mathematical expressions for radiation reaction employs advanced potentials,¹³ which this formulation excludes as a persistent feature, a new physical model of radiation reaction is needed.

Assuming that the universe as a whole is electrically neutral, a particular charge will induce among all other charges a coincident virtual negative image charge. Radiation reaction is assumed to be the interaction of a charge with its own induced image. The equations of motion for this system are (2.9), where particle 1 is the charge and particle 2 is its image. Solving this system is made easier by the following. One, to first order, \mathbf{x}_1 equals \mathbf{x}_2 (modulo effects of reaction lag). Two, the interaction from the induced image implodes on the charge as if from an oppositely charged concentric spherical shell. To an accelerated charge, in its own frame, this interaction is identical to that of a pre-counter-accelerated shell, which in turn, is identical to the sign-changed, time-reversed effect of the charge itself; i. e., $F_2|_{\text{ret}}$ equals $F_1|_{\text{adv}}$. With this substitution, Eqs. (2.9) can be added to give (note: $e_2 = -e_1$)

$$m(\ddot{\mathbf{x}}_1)^\mu = (e/2c)(F_1|_{\text{ret}} - F_1|_{\text{adv}})^{\mu\nu}(\dot{\mathbf{x}}_1)_\nu. \quad (4.1)$$

This equation is precisely the starting point of the derivation of an explicit form for the force of radiation reaction¹⁴ which is not herein reiterated.

5. COMMENTS AND CONCLUSIONS

The Lagrangians (2.8) and (3.1) both employ a notational gimmick that can lead to confusion. The problem is that in both formalisms two types of integrations appear, each with a distinct function. In (2.7) the integration on τ and in (3.2) the integrations on τ_j belong to the variational principle; whereas, the remaining integrations really are superfluous. They are part of

a notational gimmick used to express Lienard–Wiechert potentials in an elegant form by exploiting the properties of the Dirac delta function.¹⁵ In fact, the delta function can be expanded and the integrations over the dummy variables τ_k in (3.1) and τ' in (2.8) executed to write these Lagrangians in a more transparent form before executing the variation. This form would preclude confusion regarding the distinct roles of the various τ 's and integrations, albeit at a cost in elegance.

The structure of differential-difference equations, such as (2.9), is such that there is not a unique orbit through each point in phase space. This fact is another facet of the requirement for more than Cauchy initial data. A consequence of this fact is that there is no surface, spacelike or otherwise, perpendicular to all orbits whose evolution is regulated by the dynamics such that it could be parameterized by a single variable. This has led to the belief that a single variable cannot be used to parameterize all orbits; however, when each orbit is regarded independently, no problems arise for lack of such a surface or other simple correlation between filar marks on world lines.

The essential difference between various formulations of the electromagnetic two-body problem is in the selection of the interactions. Any formulation in which the interactions are derived from Lienard–Wiechert potentials is consistent with Maxwell's equations. In this formulation the mathematical formalism selects only retarded interaction except when one particle punctures the future light cone of the other to become free while the latter "sees" retarded and advanced interactions. Further study may show, however, that this transition effect cannot occur in realistic (many-body) circumstances. But, if it does occur, it might confirm the validity of this formulation. Confirmation can in principle also be obtained by comparing observed with computed world lines (when the formalism permits), but again many-body or quantum effects would probably intervene to make this difficult or ambiguous.

In conclusion, this article describes a formulation for electromagnetic force whose equations of motion can be integrated by a local scheme (i. e., mechanically) and which reveals a potential novel physical effect manifested by straight segments of the world lines of interacting particles. Moreover, this formulation affords new insights into radiation reaction.

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Error bounds for the complex-coordinate method

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In this paper we derive calculable bounds for the error in two-body *s*-wave scattering calculations done by the complex-coordinate method. In the process we derive a bound on the error in the Born approximation. The utility of the results is discussed in light of simple examples.

INTRODUCTION

Variational methods have long provided one of the most accurate means of performing numerical calculations for potential scattering. Since most calculations involve expanding in a square-integrable set of trial functions, the incident and scattered waves must be put into the problem explicitly. For most problems the initial state is relatively simple, so for those problems having simple final states, the necessity of explicitly including the final state boundary condition in the problem presents no particular hardship. For those problems having complicated final states (especially three-body states), however, the labor involved becomes prohibitive.

These facts have led to an interest in developing variation techniques which avoid the necessity of explicitly representing the scattered wave. These techniques involve working for complex values of the energy, the momentum, or the spatial coordinate.

In this paper we will consider certain formal properties of one of these methods—the complex-coordinate method.¹ We will derive calculable bounds on the error in the approximate *T* matrix resulting from an application of the complex-coordinate method, assuming certain restrictions on the potential involved. Although, as mentioned above, the method was developed for use in complex scattering problems, in this paper we will consider only the *s*-wave scattering of two simple particles interacting via a local potential $V(r)$.

We will assume that $V(r)$ is an analytic function of r in the domain $|\arg r| < \alpha$, and that for sufficiently large $|r|$ in this domain $|V(r)| < \exp(-\epsilon|r|)$. We also assume that $V(r)$ is real for real r . With these assumptions the *T* matrix has been shown to satisfy the following stationary expression¹:

$$\langle p | Tp \rangle = \langle p | Vp \rangle + \theta^* \langle p \theta | V_\theta \chi \rangle + \theta^* \langle \chi^* | [V_\theta | p \theta^*] - \theta^* \langle \chi^* | (E + \theta^2 d^2/dr^2 - V_\theta) \chi \rangle. \quad (1)$$

In this expression $|p\rangle = (\sin pr)/p$, $V_\theta = V(r\theta^*)$, and χ is a trial function to be varied subject to the restrictions that it be square-integrable and lie in the domain of definition of the relevant operators. θ is a complex number of unit magnitude satisfying the restriction

$$0 < \arg \theta < \min[\alpha, \tan^{-1}(\epsilon/p)]. \quad (2)$$

Numerical values for the *T* matrix are obtained by the

following procedure: Expand χ in a complete set of functions f_i keeping N terms:

$$\chi = \sum_{i=1}^N a_i f_i, \quad (3)$$

where the a_i are numbers to be solved for. This formula for χ is substituted into Eq. (1) and the implied integrations are performed producing a bilinear form in the a_i . By setting the partial derivative of this form with respect to each a_i equal to zero, an inhomogeneous set of linear equations is obtained and subsequently solved for the a_i . These values of a_i are then used to calculate an approximate value of *T* by Eqs. (3) and (1).

It is easy to see that the value of *T* derived by the method of the previous paragraph can be written as follows¹:

$$\langle p | Tp \rangle = \langle p | Vp \rangle + \theta^* \langle V_\theta^* [p \theta] | P^N [E + P^N (\theta^2 d^2/dr^2 - V_\theta) P^N]^{-1} P^N V_\theta [p \theta^*] \rangle \quad (4)$$

where P^N is the projection operator which projects onto the space spanned by the first N f_i 's.

In the next section we will derive a bound on the difference between the right-hand side of Eq. (4) and the exact *T* matrix under the assumption that we know a bound for $\|(E - \theta^2 d^2/dr^2 - V_\theta)^{-1}\|$. In the following section we will derive a bound on this expression for more restrictive classes of potentials.

ERROR BOUNDS

Throughout this section we will assume that the following relation holds:

$$\|(E + \theta^2 d^2/dr^2 - V_\theta)^{-1}\| \leq \Delta. \quad (5)$$

In the following section we will derive expressions for Δ under various assumptions on V .

If in Eq. (4) we replace P^N by $\mathbf{1}$, the resulting equation for *T* is exact. The error in the approximate *T* matrix is therefore given by

$$\begin{aligned} \mathcal{E} = & \left\langle V_\theta^* [p \theta] \left| \left\{ \left(E - \theta^2 \frac{d^2}{dr^2} - V_\theta \right)^{-1} \right. \right. \right. \\ & \left. \left. \left. - P^N \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} P^N \right\} V_\theta [p \theta^*] \right\rangle \\ & \times \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} P^N \left\{ V_\theta [p \theta^*] \right\}. \end{aligned} \quad (6)$$

We define a vector Σ to be:

$$\Sigma \equiv \left\{ \mathbf{1} - \left(E + \theta^2 \frac{d^2}{dr^2} - V_\theta \right) \right.$$

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$$\times P^N E + P^N \theta^2 \frac{d^2}{dr^2} - V_\theta P^N \left. P^N \right| V_\theta [p\theta^*] . \quad (7)$$

Σ can be constructed very simple from the information obtained in generating the approximate T matrix. Using this definition and Eq. (5), we find, applying the Schwartz inequality to Eq. (6),

$$|\mathcal{E}| \leq |V_\theta^*[p\theta]| |\Sigma| \Delta. \quad (8)$$

The first two factors on the right-hand side of this inequality can be computed with available information. If a value of Δ is provided, Eq. (8) therefore represents

$$\begin{aligned} |\Sigma|^2 = & \langle V[p\theta^*] | V[p\theta^*] \rangle - \left\langle \left(E + \theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} V[p\theta^*] | V_\theta [p\theta^*] \right\rangle \\ & - \left\langle V_\theta [p\theta^*] \left| \left(E + \theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} V_\theta [p\theta^*] \right\rangle + \left\langle \left(E + \theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right. \\ & \left. \times \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} V_\theta [p\theta^*] \left| \left(E + \theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \left[E + P^N \left(\theta^2 \frac{d^2}{dr^2} - V_\theta \right) P^N \right]^{-1} V_\theta [p\theta^*] \right\rangle. \quad (10) \end{aligned}$$

If the complex-coordinate method is to work well, it is reasonable to expect that the first three terms of Eq. (10) approach $\langle V_\theta [p\theta^*] | V_\theta [p\theta^*] \rangle$ fairly rapidly. Heuristically speaking this depends on the rate of convergence of generalized Fourier series for the wave function in terms of the f_i 's. The last term in Eq. (10) requires more careful examination.

We call the last term of Eq. (10) δ and write

$$\begin{aligned} \delta = & \langle V_\theta [p\theta^*] | P^N V_\theta [p\theta^*] \rangle + \langle (d^2/dr^2)\phi | Q^N (d^2/dr^2)\phi \rangle \\ & + \langle V_\theta \phi | Q^N V_\theta \phi \rangle - \langle V_\theta \phi | Q^N (d^2/dr^2)\phi \rangle \\ & - \langle Q^N (d^2/dr^2)\phi | V_\theta \phi \rangle, \quad (11) \end{aligned}$$

where $Q^N \equiv 1 - P^N$ and $\phi \equiv P^N [E + P^N (\theta^2 d^2/dr^2 - V_\theta) P^N]^{-1} \times |V_\theta [p\theta^*]\rangle$.

Assuming we have not made an inane choice of f 's, the first term in Eq. (11) will rapidly approach $\langle V_\theta [p\theta^*] | V_\theta [p\theta^*] \rangle$. Thus, if we expect $|\mathcal{E}|$ to go to zero, we must have the last four terms in Eq. (11) go to zero. Again speaking heuristically we expect these terms to decrease rapidly in magnitude only if the f 's can easily represent not only the wave function, but also $(d^2/dr^2)f_i$ and $V_\theta f_i$. In general this will be a substantially more restrictive requirement.

Only experience can effectively test the usefulness of the bound given by Eq. (8), but the arguments at the last paragraphs do not appear particularly hopeful. It is likely that there exist examples for which the complex-coordinate method converges quite nicely but for which the right-hand side of Eq. (9) does not approach zero. This does not mean to say, of course, that even for such cases the bound might not be useful. The bound on the Born approximation does not depend on the f 's, and it is hard to guess to what extent Eq. (9) may be valuable.

In light of these remarks we consider the example

$$\begin{aligned} V(r) = & -\exp(-r), \\ f_i = & \left(\frac{i+1}{i} \right)^{1/2} \exp(-r/2) \sum_{k=1}^i \binom{i}{k} k \frac{(-r)^k}{(k+1)!}. \quad (12) \end{aligned}$$

a computable bound on the error in the N th approximation by the complex-coordinate method.

It is interesting to note that since the "zerth order" approximation in the complex-coordinate method is the Born approximation, we have derived a bound on the error in Born calculations. If we let \mathcal{E}_B be the error in the Born approximation for the potential V , we find (setting $\Sigma = |V_\theta^*[p\theta]\rangle$):

$$|\mathcal{E}_B| \leq |V_\theta^*[p\theta]|^2 \Delta. \quad (9)$$

We now wish to consider the quantity $|\Sigma|$ in more detail. We start by writing

This set of f 's is complete and orthonormal. The wave-function χ [by this we mean the function for which Eq. (1) is stationary] vanishes at the origin and the Fourier series for it in terms of the f 's converges very rapidly. We therefore expect that the complex-coordinate method will work quite well, and this expectation is easily verified. The functions $(d^2/dr^2)f_i$ do not vanish at the origin and the generalized Fourier series for them converge only like $1/N$, N being the number of terms. For this example $V_\theta f$ is well approximated by a series of f 's, but this would not have been the case if we had chosen a Yukawa potential. The function δ of Eq. (11) converges very slowly in this example, and the error bound of Eq. (8) is much larger than the actual error.

The results for the bound on the error in the Born approximation given by Eq. (9) are harder to interpret. We will show in the next section that if p is greater than 1, a bound on Δ is given by

$$\Delta \leq 1/\sin 2\alpha (p^2 - 1), \quad (13)$$

where

$$\theta = \exp(i\alpha),$$

Using this we find:

$$|\mathcal{E}_B| \leq 1/4(p^2 - 1)(p^2 + 1)(1 - p^2 \tan^2 \alpha) \cos^3 \alpha \sin 2\alpha. \quad (14)$$

We choose α to minimize this expression and compute the values for \mathcal{E}_B given in Table I. In this table Amp is

TABLE I. A comparison of the error in the Born approximation amplitude with the error bound for the potential $V = e^{-r}$.

P	Amp	B	E	\mathcal{E}_B	R
1.4	0.208 + 0.067i	0.226	0.0694	0.219	3.16
1.7	0.149 + 0.041i	0.159	0.0418	0.0948	2.26
2.0	0.112 + 0.026i	0.118	0.0270	0.0517	1.91
2.3	0.0864 + 0.0179i	0.0903	0.0183	0.0318	1.73
2.6	0.0689 + 0.0127i	0.0713	0.0130	0.0211	1.63
2.9	0.0561 + 0.0094i	0.0577	0.0095	0.0148	1.55

TABLE II. A comparison of the error in the phase shift obtained from two methods of unitarizing the Born approximation with the allowed range given by the error bound.

P	δ	δ_1	δ_2	δ_{\max}	δ_{\min}
1.4	0.3112	0.2823	0.3067	0.56	0.01
1.7	0.2658	0.2481	0.2644	0.39	0.11
2.0	0.2314	0.2110	0.2311	0.30	0.14
2.3	0.2046	0.2967	0.2047	0.25	0.14
2.6	0.1831	0.1776	0.1834	0.22	0.14
2.9	0.1656	0.1617	0.1659	0.19	0.13

the exact scattering amplitude, B is the Born approximation, E is the absolute value of the error in the Born approximation, and R is the ratio of E to the bound \mathcal{E}_B . As the Born approximation becomes better for larger p the bound also becomes better. For values of p larger than 2 the bound on the error is always less than twice the magnitude of the actual error, which seems quite acceptable.

Table I and the discussion of the previous paragraph probably overstate the value of \mathcal{E}_B for the particular example considered. The reason for this is that no use was made of the knowledge that the scattering amplitude must satisfy the requirements of unitarity. Presumably anyone trying to solve this problem would compute a phase shift, rather than a scattering amplitude, as a means of unitarizing the Born approximation.

If we draw a circle of radius \mathcal{E}_B around the Born approximation, the intersection of this circle with the curve $(1/p)[\exp(i\delta)\sin\delta]$ will determine a maximum and minimum value for δ . These values are listed as δ_{\max} and δ_{\min} in Table II. δ_1 and δ_2 are approximate values of δ obtained from two different ways of unitarizing the Born calculation. δ_1 is the closest point on the curve $(1/p)[\exp(i\delta)\sin\delta]$ to the value of the Born amplitude. δ_2 is the R -matrix approximation obtained by setting $\tan\delta_2 = pB$.

Clearly, the approximate δ represented by δ_2 is much the better of the two. Even at $P = 2.9$ the range of values between δ_{\max} and δ_{\min} is very large compared with the actual error in the approximation δ_2 . The values of δ_1 are not as accurate as those of δ_2 and for these calculations the actual error is about 10 percent of the value suggested by δ_{\max} and δ_{\min} . This bound is perhaps good enough to be interesting, but is not nearly as good as the bound for the scattering amplitude.

If the theorems in this paper are generalized to include those cases for which unitarity cannot be as usefully applied (scattering of particles with internal structure, many-body scattering, complex potentials, etc.), it may be that a bound such as that of Eq. (9) would actually prove useful.

EXPRESSIONS FOR Δ

In this section we derive expressions for Δ of Eq. (5) under various assumptions on V . We begin by showing that such a bound must exist. To do this we must learn something about the spectrum of the operator:

$$H_\theta \equiv -\frac{d^2}{dr^2} + \theta^{*2} V_\theta. \quad (15)$$

From the obvious identity

$$\left(\lambda + \frac{d^2}{dr^2} - \theta^{*2} V_\theta\right)^{-1} = \theta^2 \left(\theta^2 \lambda + \theta^2 \frac{d^2}{dr^2} - V\right)^{-1} \quad (16)$$

we see that if λ is in the resolvent set of H_θ , then $\theta^2 \lambda$ is in the resolvent set of:

$$-\theta^2 \frac{d^2}{dr^2} + V_\theta. \quad (17)$$

We now wish to consider the Jost function² $f_\theta(\rho)$ for the operator $H_\theta - \rho^2$. The assumptions we have made about V assure that $f_\theta(\rho)$ will be analytic in the domain $\text{Im}\rho > -\epsilon/2$. Furthermore, for all values of ρ which satisfy this condition, $f_\theta(\rho)$ can be expanded in a convergent series of the form

$$f_\theta(\rho) = 1 + \sum g_n(\rho),$$

where the g_n are integrals of the form

$$g_n = \frac{1}{(2i\rho)^n} \int_0^\infty dz_1 [\exp(2iz_1\rho) - 1] \theta^{*2} V(\theta^* z_1) \int_{z_1}^\infty dz_2 \times \{\exp[2i\rho(z_2 - z_1)] - 1\} \theta^{*2} V(\theta^* z_2) \dots \times \int_{z_{n-1}}^\infty dz_n \{\exp[2i\rho(z_n - z_{n-1})] - 1\} \theta^* V(\theta^* z_n). \quad (18)$$

We change the integration variable $z_i \rightarrow \theta y_i$ to obtain

$$g_n = \frac{1}{(2i\rho\theta)^n} \int_0^\infty dy_1 [\exp(2i\rho\theta y_1) - 1] V(y_1) \int_{y_1}^\infty dy_2 \times \{\exp[2i\rho\theta(y_2 - y_1)] - 1\} V(y_2) \dots \int_{y_{n-1}}^\infty dy_n \times \{\exp[2i\rho\theta(y_n - y_{n-1})] - 1\} V(y_n). \quad (19)$$

This is the g_n appropriate to the expansion of $f_1(\theta\rho)$. We have thus shown that for the domain where $\text{Im}\rho$ and $\text{Im}\theta\rho$ are both greater than $-\epsilon/2$ we have

$$f_\theta(\rho) = f_1(\rho\theta). \quad (20)$$

For $\theta = 1$, H_θ is a self-adjoint operator whose Jost function cannot be zero for real positive values of the argument. Using this fact and Eq. (20), we find that

$$f_\theta(\rho\theta^*) = f_1(\rho) \quad (21)$$

cannot be zero for real positive ρ as long as θ and ρ are such as to satisfy the condition leading to Eq. (20). We can assure the validity of Eq. (20) by imposing the further restriction on θ : $\arg\theta < \sin^{-1}\epsilon/\rho$ [see Eq. (2)].

For operators of the H_θ type all positive real numbers will be in the continuous spectrum. A nonreal number λ having a positive real part will be in the point spectrum of H_θ if $f_\theta(\sqrt{\lambda}) = 0$, and in the resolvent set otherwise.³ Equation (21) shows that λ of the form $\rho^2\theta^{*2}$, where ρ is real, are in the resolvent set of H_θ . Combining this result with Eqs. (16) and (5), we have proved that

$$\|(E + \theta^2 d^2/dr^2 - V_\theta)^{-1}\| \quad (22)$$

is finite and thus the bound on Δ which we seek must exist.

To find a calculable bound for Δ , it will be necessary to impose more restrictions on V . One case for which

we can give such a bound is $|\text{Im} \theta^{*2} V(\theta^* r)| < \infty$. For this case we define the operator

$$H_R \equiv -\frac{d^2}{dr^2} + \text{Re}[\theta^{*2} V(\theta^* r)]. \quad (23)$$

H_R is a self-adjoint operator and therefore has no spectral points off the real axis. Thus we have

$$\|(\theta^{*2} E - H_R)^{-1}\| < 1/|\text{Im} \theta^{*2} E|. \quad (24)$$

If $\|\text{Im} \theta^{*2} V(\theta^* r)\| = \max |\text{Im} \theta^{*2} V(\theta^* r)| < \text{Im} \theta^{*2} E$, we have⁴

$$\begin{aligned} \Delta &= \|(E + \theta^2 d^2/dr^2 - V_\theta)^{-1}\| = \|(\theta^{*2} E + d^2/dr^2 - \theta^{*2} V_\theta)^{-1}\| \\ &\leq (|\text{Im}(\theta^{*2} E)| - \|\text{Im} \theta^{*2} V(\theta^* r)\|)^{-1}. \end{aligned} \quad (25)$$

In Eqs. (24) and (25) we have assumed E is real. Equation (25) provides the bound on Δ we desire. If the potential is an analytic function of r and satisfies the rest of the requirements of this paper, it is clear that the bound of Eq. (25) will apply for sufficiently high energy.

We will now consider the bound given by Eq. (25) in the special case $V = -\exp(-r)$. We set $\theta = \exp(i\alpha)$ and find

$$\text{Im} \theta^{*2} V(\theta^* r) = \exp(-2i\alpha) \exp[\exp(-i\alpha)r], \quad (26)$$

or

$$\begin{aligned} |\text{Im} \theta^{*2} V(\theta^* r)| &= |\exp(-r \cos \alpha)(\cos 2\alpha \sin(r \sin \alpha) \\ &\quad - \sin 2\alpha \cos(r \sin \alpha))| \leq \sin 2\alpha. \end{aligned} \quad (27)$$

Substituting this result into Eq. (25), we find

$$\Delta \leq 1/\sin 2\alpha(p^2 - 1), \quad p > 1, \quad (28)$$

where p is the momentum. This relation is the same as Eq. (13) of the previous section.

CONCLUSIONS

We have given formulas for a calculable bound on the error in scattering calculations done by the complex-coordinate method. We expect that similar results can be given for more complicated (realistic) problems in which case the error bound might provide useful information. If experience proves the error bound to be uselessly imprecise, some may still find its existence to be of interest. As a final remark we point out that even for those potentials which satisfy our requirements, Eq. (8) cannot be used to prove the convergence of the method. The reason is that we cannot bound the spectrum of the projected operators away from the real axis. If, in addition to the requirements already imposed, we insist that the potential have a sufficiently small derivative⁵ on the real axis, then it is easy to bound the resolvents of the projected operators, and Eq. (8) can be used to prove the convergence of the method to the correct answer as N becomes large. This condition on the derivative of the potential does not appear to us to be very natural, and we believe that it will be possible to prove the convergence of the method without such an assumption.

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Lower hybrid solitary waves

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It is found that, in a magnetized plasma, finite amplitude lower hybrid waves can propagate as solitons consisting of localized density cavities together with doublets of electric field spikes. An analytical expression, as well as the corresponding evolution equation, are derived for the small amplitude limit. Such solitons can also exist for many other waves having similar dispersive and nonlinear characteristics.

I. INTRODUCTION

It is well known that nonlinear dispersive waves can propagate in the form of localized pulses known as solitons.¹ In particular, the Korteweg-de Vries (KdV) equation and its soliton solutions have been studied extensively for waves in various branches of physics. In this paper, we investigate a new type of soliton, which is associated with waves having a linear dispersion relation different from that of the KdV equation

As a concrete example, we shall consider nonlinear lower hybrid waves² propagating perpendicular to an external magnetic field in a plasma. The derivation and results presented here are applicable to many other waves having similar dispersive and nonlinear properties.

It is found that such waves can propagate as solitary pulses. The latter consist of localized density cavities together with spiky electric fields. An analytical expression is derived for small amplitude solitons. We also obtain by means of an appropriate scaling scheme an equation governing the evolution of the latter.

II. DERIVATION OF EQUATIONS

For simplicity, we shall consider a lower hybrid wave pulse moving exactly perpendicular to the external magnetic field $B_0 \hat{z}$. The appropriate equations describing such a wave are

$$\partial_t n_j + \partial_x (n_j v_{xj}) = 0, \quad (1)$$

$$\partial_t v_{xj} + v_{xj} \partial_x v_{xj} = -v_{Tj}^2 \partial_x \ln(n_j/n_0) - (q_j/m_j) \partial_x \phi + \Omega_j v_{yj}, \quad (2)$$

$$\partial_t v_{yj} + v_{xj} \partial_x v_{yj} = -\Omega_j v_{xj}, \quad (3)$$

$$n_i = n_e, \quad (4)$$

where $j = i, e$; $v_{Tj} = (T_j/m_j)^{1/2}$, $\Omega_j = e_j B_0/m_j c$, and $q_i = -q_e = e$. Equation (4) corresponds to the quasineutrality condition. The wave propagates in the x direction. When linearized, Eqs. (1)–(4) lead to the dispersion relation

$$\omega^2 = \Omega_e \Omega_i (1 + k_x^2 v_{Tj}^2 / \Omega_e^2), \quad (5)$$

for lower hybrid wave propagation perpendicular to an external magnetic field. Here $v_T^2 = (T_i + T_e)/m_e$. Assuming a steady state ($\partial_\tau = 0$) in the moving frame

$\tau = t$, $\xi = x - Vt$, we obtain from (1)

$$v_{xj} - V = -n_0 V / n_j. \quad (6)$$

The plasma is assumed to be at rest at infinity, where $n_j = n_0$.

Eliminating v_{xj} and v_{yj} from (2), (3), and (6), we get

$$\begin{aligned} \partial_{\xi\xi} [n_0^2 V^2 / 2n_e^2 + v_{Te}^2 \ln(n_e/n_0) - e\phi/m_e] \\ = \Omega_e^2 (n_e/n_0 - 1) \end{aligned} \quad (7)$$

and

$$\partial_{\xi\xi} [n_0^2 V^2 / 2n_i^2 + v_{Ti}^2 \ln(n_i/n_0) + e\phi/m_i] = 0 \quad (8)$$

for electrons and ions respectively. The ions are assumed to be unmagnetized ($\Omega_i = 0$).

For convenience, in the following we nondimensionalize the quantities ξ , n_j , $e\phi$, and V by an effective Larmor radius $R_e = v_{Te}/\Omega_e$, the unperturbed number density n_0 , the electron temperature T_e and the ion-acoustic speed $c_s = [(T_i + T_e)/m_i]^{1/2}$, respectively. Integration of (8) yields

$$\phi = -V^2/2n_i^2 + V^2/2 - (T_i/T_e) \ln n_i, \quad (9)$$

where we have used the conditions $\phi = 0$ and $n_i = 1$ at infinity.

Substituting (9) into (7), and using (4), we obtain

$$\partial_{\xi\xi} (\ln n + V^2/2n^2) = n - 1, \quad (10)$$

where $n = n_i = n_e$, and we have assumed $m_e/m_i \ll 1$. The last condition amounts to neglecting electron inertia.

Equation (10) can be integrated once by first multiplying both sides by $\partial_\xi (\ln n + V^2/2n^2)$. One obtains

$$\begin{aligned} \frac{1}{2} [\partial_\xi (\ln n + V^2/2n^2)]^2 \\ = n + V^2/n - \ln n - V^2/2n^2 - 1 - V^2/2, \end{aligned} \quad (11)$$

where the boundary conditions at infinity have been used. Equation (11) can now be put into a form resembling the energy integral of a classical particle with zero total energy. Accordingly, one obtains

$$\begin{aligned} \frac{1}{2} (\partial_\xi n)^2 = -\Psi(n) \\ = n^4 \left[\frac{n^3 - n^2 + V^2 n - n^2 \ln n - V^2 n^2/2 - V^2/2}{(n^2 - V^2)^2} \right]. \end{aligned} \quad (12)$$

The potential $\Psi(n)$ can be analyzed in the usual manner for the existence of solitary solutions of (12).

III. SOLITON SOLUTION

It can be shown that there exists $n = n_M < 1$, given by

$$n_M^3 - n_M^2 \ln n_M - n_M^2 = V^2(\frac{1}{2} - n_M + n_M^2/2), \quad (13)$$

such that $\Psi(n_M) = 0$ and $\Psi'(n_M) < 0$. One can also show that $\Psi(1) = \Psi'(1) = 0$ and $\Psi(n) < 0$ if $V < 1$ and $n_M < n < 1$. Furthermore, we note that $\Psi(n) \rightarrow -\infty$ at $n = n_b = V$, and $n_m < n_b < 1$ (see Fig. 1). The typical profile of $\Psi(n)$ is shown in Fig. 2.

It is of interest³ to look at the behavior of a classical particle in a potential well resembling that in Fig. 2. Accordingly, Ψ is the potential energy of the particle, ξ and n are the time and space variables respectively. A particle with zero total energy would start from $n = 1$, take infinite time to leave this point, and reach $n = n_b$, where it attains infinite speed. After n_b , it slows down and eventually arrives at n_M , where it is reflected by the potential wall. The particle then returns to the point $n = 1$ in a symmetrical manner.

From the above discussion, we see³ that the solution of (11) consists of a localized density depression ($n \leq 1$) which is symmetrical about the point of minimum density. This solution is peculiar in that it contains two points at which the density gradient is infinite, although the density itself is continuous (see Fig. 3). Since $E = -\partial_\xi \phi = (V^2/2n^2)\partial_\xi n$, the electric field associated with the soliton has a profile consisting of two adjacent spikes, one positive and one negative.

By choosing other boundary conditions, one can construct analogous cnoidal wave solutions with spiky electric fields.

IV. SMALL AMPLITUDE LIMIT

In this section, we show that an analytical expression can be obtained for the case of a small amplitude ($n \approx 1$) near-sonic ($V \approx 1$) lower hybrid soliton.

Consider the limit $\delta n = 1 - n \ll 1$, $\delta V = 1 - V \ll 1$, such that $\delta n = O(\delta V)$. One obtains from (12),

$$(\partial_\xi \delta n)^2 = \frac{\delta V n^2 - 2\delta n^3/3}{2(\delta V - \delta n)^2}. \quad (14)$$

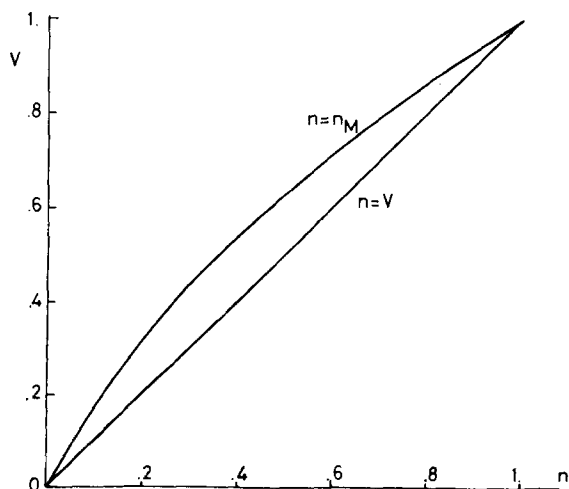


FIG. 1. The curves $n = n_M$ and $n = n_b = V$. Note that for any given V , n_M lies to the left of n_b .

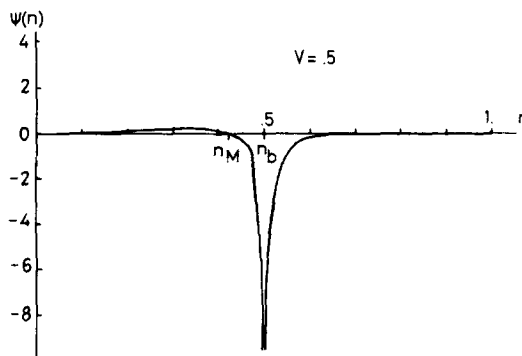


FIG. 2. The potential $\Psi(n)$ for the case $V = 0.5$.

Equation (14) can also be derived from (1)–(4) by means of an appropriate ordering scheme.

Integration of (14) yields

$$\delta n = \frac{3\delta V}{2} \operatorname{sech}^2 \left[\frac{|\xi| - \xi_0}{2(2\delta V)^{1/2}} + \left(3 - 2 \frac{\delta n}{\delta V} \right)^{1/2} \right], \quad (15)$$

where $\xi_0 = 0$ for $0 < |\xi| < \xi_b$, and $\xi_0 = 2\xi_b$ otherwise. We have defined

$$\xi_b = 2(2\delta V)^{1/2} [1 + \operatorname{sech}^{-1}(\frac{2}{3})]^{1/2}. \quad (16)$$

Note that (15) is a transcendental equation for δn . In Fig. 3 the solution is plotted for two values of V . The arrows indicate the locations where $n = n(\xi_b)$.

It is of interest to derive a time dependent equation governing the evolution of the small amplitude solitons. The ordering necessary for deriving this equation can easily be deduced from the stationary solution (15).⁴

In addition to the dimensionless variables introduced earlier, we nondimensionalize time by $(\Omega_i \Omega_e)^{-1/2}$, and introduce the stretched independent variables $\eta = \epsilon^{-1/2}(x - t)$, $\tau = \epsilon^{1/2}t$, where $\epsilon = (m_e/m_i)^{1/2} \ll 1$ is a small parameter. Thus, we use a frame which is moving with the ion-acoustic speed c_s . For the dependent

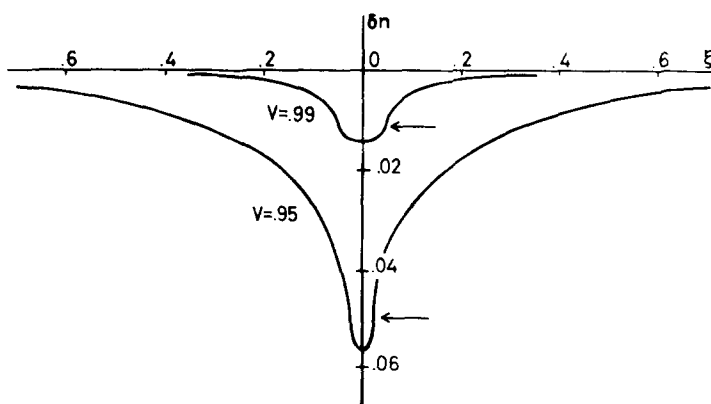


FIG. 3. Density cavities for $V = 0.95$ and 0.99 . The arrows indicate the locations where the density gradient is infinite.

variables, we make the expansions

$$\begin{aligned} n_j &= 1 + \epsilon n_{j1} + \epsilon^2 n_{j2} + \dots, \\ v_{jx} &= \epsilon v_{jx1} + \epsilon^2 v_{jx2} + \dots, \\ v_{ey} &= \epsilon^{1/2} v_{ey1} + \epsilon^{3/2} v_{ey2} + \dots, \\ \phi &= \epsilon \phi_1 + \epsilon^2 \phi_2 + \dots. \end{aligned} \quad (17)$$

After some algebra, we obtain from (1)–(4) the following equation for n_1 ,

$$-2\partial_{\tau\tau} n_1 - \partial_{\eta\eta} n_1^2 + n_1 = 0. \quad (18)$$

It can be shown that a steady state solution of (18) is given by (15). On the other hand, Eq. (18) leads to the linear dispersion relation

$$\omega = k_x c_s + (\Omega_i \Omega_e)^{1/2} / 2k_x R_e, \quad (19)$$

which agrees with that of a linear lower hybrid wave propagating perpendicular to the external magnetic field near the sound speed.

In the small amplitude limit considered here, the typical phase velocity of the waves is near the sound speed. In view that finite electron Larmor radius effects have been neglected [i. e., $k_x^2 R_e^2 \ll 1$, where $R_e = v_{Te} / \Omega_e = R(1 + T_i/T_e)^{-1/2}$], we require $T_i \gg T_e$ for consistency. In the microscopic picture, the latter condition puts a restriction on the possible form of the ion velocity distribution function, otherwise ion Landau damping effects might dominate, as is in the case of Maxwellian distribution.

V. DISCUSSION

The soliton discussed in this paper consists of a solitary moving density cavity with two points at which the electric field is infinite. It is expected that in reality, effects such as two-dimensionality, charge separation, particle acceleration and trapping, etc. which have been neglected in the present analysis, should limit the amplitude of these electric field spikes without changing the overall picture given here.

We note that by choosing a strictly one-dimensional propagation perpendicular to the external magnetic field, we have neglected the parallel electron dynamics as well as the $E \times B$ nonlinearities, both of which are known to be important in smaller amplitude lower hybrid wave propagation.

Similar solitons can easily be obtained for electron plasma waves,⁵ upper hybrid waves, electrostatic ion-cyclotron waves, drift waves, etc., whose linear dispersion relations are of the form $\omega^2 = a + bk^2$. In this respect, Eq. (18) corresponds to the case $\omega \approx b^{1/2}k$, so that $\omega \approx b^{1/2}k + a/2b^{1/2}k$. It is of interest to note the difference between (18) and the Korteweg–de Vries equation, whose linear dispersion relation is $\omega = ak + bk^3$ and is derived with a different scaling of the time, space, and amplitude variables, although in both cases the equations describe nonlinear dispersive waves.

The solitons discussed here can be of practical interest. One may look upon such pulses as condensates of waves in physical space. In a turbulent plasma, where wave–wave interactions are the main transport mechanism, the existence of these condensates can significantly alter the transport properties of the plasma and hence the turbulent spectrum.

ACKNOWLEDGMENT

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High-precision determination of the critical screening length for the static screened Coulomb potential

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By a combination of analytical and numerical methods, it is determined that the critical screening length for two particles interacting through an attractive static screened Coulomb potential lies between $0.8399032a_0$ and $0.8399039a_0$, where a_0 is the Bohr radius.

The attractive static screened Coulomb potential (SSCP)

$$V(r) = -e^2 e^{-r/d}/r, \quad (1)$$

where d is a screening length, is of interest in many areas of physics. For a cross section of references in which the properties of this potential have been investigated, reference may be made to Refs. 1–3 and to the references quoted therein.

A quantity of special interest, for two particles interacting through an attractive SSCP, is the critical screening length, d_c , for the ground state. For $d < d_c$, the eigenstate is not bound, i. e., it cannot be formed with negative energy. The critical screening length, for the ground state has been calculated by a variety of techniques.^{1,4–13} In this paper we present a high-precision value for this length using a method due to Trubnikov and Yavlinskii.⁹

For the potential (1), the Schrödinger equation can be reduced to the form

$$u''(x) = -\beta(e^{-x}/x)u(x) \quad (2)$$

where $u = \psi r$, $x = r/d$, and $\beta = 2d/a_0$, a_0 being the Bohr radius. The boundary conditions are

$$u(0) = 0, \quad (3a)$$

$$u(\infty) = \text{const} = 1. \quad (3b)$$

Trubnikov and Yavlinskii⁹ sought the solution in the form of a series in β :

$$u(x) = 1 + \sum_{n=1}^{\infty} (-\beta)^n u_n(x), \quad (4)$$

where

$$u_n(x) = \int_1^{\infty} \dots \int_1^{\infty} \frac{\exp[-x(t_1 + t_2 + \dots + t_n)] dt_1 dt_2 \dots dt_n}{t_1^2(t_1 + t_2)^2 \dots (t_1 + t_2 + t_3 + \dots + t_n)^2}. \quad (5)$$

Expression (4) satisfies the differential equation (2) and the condition (3b). The condition (3a) will also be satisfied if β is the root of the equation

$$1 + \sum_{n=1}^{\infty} (-\beta)^n a_n = 0, \quad (6)$$

where the coefficients a_n are determined by

$$a_n = u_n(0) = \int_1^{\infty} \frac{dt_1}{t_1^2} \int_{1+t_1}^{\infty} \frac{dt_2}{t_2^2} \dots \int_{1+t_{n-1}}^{\infty} \frac{dt_n}{t_n^2}. \quad (7)$$

The series (6) converges rapidly. By retaining an increasing number of terms in series (6), one can improve the degree of accuracy in the determination of β_c .

The first three coefficients can be readily evaluated and these are as follows:

$$a_1 = 1,$$

$$a_2 = 1 - \ln 2,$$

and

$$a_3 = 1 + \ln 2 - (3/2)\ln 3.$$

Trubnikov and Yavlinskii⁹ determined a_4 to two significant figures and a_5 to one significant figure, by numerical integration. Their calculated value of d_c/a_0 is 0.84.

It was found possible to reduce the iterated integrals for a_4 , a_5 , a_6 , and a_7 to single integrals and that for a_8 to a double integral. These integrals are conveniently expressed in terms of a function $\Phi(t)$, where

$$\Phi(t) = \frac{1}{2(1+t)} \ln \frac{(1+t)^{1+t}(3+t)^{3+t}}{(2+t)^{2(2+t)}}. \quad (8)$$

This is a continuous function for $t > 0$ which approaches uniformly to zero as $t \rightarrow \infty$. The explicit expressions for the coefficients a_4 to a_8 are as follows.

$$a_4 = a_3 - \int_1^{\infty} \frac{\Phi(t)}{t^2} dt,$$

$$a_5 = a_4 - \int_2^{\infty} \frac{t-2}{t-1} \frac{\Phi(t)}{t^2} dt,$$

$$a_6 = a_5 - \int_3^{\infty} \left(\frac{t-3}{t-1} + \ln \frac{t-1}{2(t-2)} \right) \frac{\Phi(t)}{t^2} dt,$$

$$a_7 = a_6 - \int_4^{\infty} \left(\frac{t-4}{t-1} + \frac{3}{2} \ln \frac{t-1}{t-2} + \frac{t-3}{2(t-1)} + \ln \frac{t-3}{2(t-3)} \right) \frac{\Phi(t)}{t^2} dt,$$

TABLE I. Critical screening lengths for the 1s state as calculated by various authors.

Author(s)	d_c/a_0
Sachs and Mayer ⁴	0.8415
Hulthén and Laurikainen ⁵	0.839910
Harris ⁶	0.87
Lovelace and Masson ⁷	0.832605
Schey and Schwartz ⁸	0.840
Trubnikov and Yavlinskii ⁹	0.84
Robinson <i>et al.</i> ¹⁰	0.84187
Rogers <i>et al.</i> ¹	0.839908
this paper	0.8399039

$$a_8 = a_7 - \int_5^\infty \frac{\Phi(t)}{t^2} dt \int_1^{t-4} \frac{1}{s^2} \frac{t-s-4}{(t-1)(s+1)} + \frac{s+3}{2(s+1)} \times \left(\ln \frac{t-1}{t-2} - \ln \frac{s+3}{s+2} \right) - \frac{t-3}{2(t-1)} \left(\ln \frac{t-3}{t-2} - \ln \frac{s+1}{s+2} \right) ds.$$

For the purpose of numerical integration, appropriate transformations were used in order to reduce the interval of integration to $(-1, 1)$. For the integral occurring in a_n , we used the transformation

$$t = 2(n-3)/u + 1.$$

The integrals were calculated numerically on an IBM 360/65 in "double precision." the results are given below:

$$a_4 = 0.390593814496 \times 10^{-2}$$

$$a_5 = 0.22135915607 \times 10^{-3}$$

$$a_6 = 0.886057280 \times 10^{-5}$$

$$a_7 = 0.26377323 \times 10^{-5},$$

and

$$a_8 = 0.6068 \times 10^{-8}.$$

The value of d_c/a_0 obtained by using these coefficients in (6) is 0.8399039. This value is compared with those obtained by previous workers in Table I.

The terms in Eq. (6) alternate in sign. Correspondingly, the calculated values of d_c/a_0 show an alternating behavior, i. e., they are alternately above and below the exact value, while converging towards it, as successively higher terms are taken into account. This property can be used to bracket the correct value of d_c/a_0 . If we retain terms only up to a_7 , we find $d_c/a_0 = 0.8399032$. Thus the exact value will lie between 0.8399032 and 0.8399039 and very likely it will be closer to the latter value than the former. Other methods which have been used in determination of d_c are not very practicable for determining such lower and upper bounds.

Dyson and Lenard¹⁴ have investigated the lower bound for the spectrum of the N -particle Hamiltonian with Coulombic interaction. The charges of the particles were of equal magnitude but of unspecified signs. These authors¹⁴ have given a number of theorems for the lower bound of the energy. In their Theorem 2, they showed

that

$$E_{\min} > -\mu N(N-1) \text{ Rydbergs,} \quad (9)$$

where $\mu = 1/\beta_c$ in terms of our notation. Dyson and Lenard¹⁴ used the approximation $\mu = 1/\sqrt{2}$ and obtained

$$E_{\min} > -[N(N-1)/\sqrt{2}] \text{ Rydbergs.} \quad (10)$$

The value of β_c determined in the present paper sharpens this limit to

$$E_{\min} > -[N(N-1)/1.6798078] \text{ Rydbergs.} \quad (11)$$

When N is large, Dyson and Lenard¹⁴ have given a better lower bound in their theorem 3:

$$E_{\min} > -52 N^{5/3} \text{ Rydbergs.} \quad (12)$$

For $N < 4 \times 10^5$, expression (10) gives better bounds than (12), while, above this value of N , the reverse is the case.

Subsequent to the work of Dyson and Lenard, there have been improvements on methods to obtain the limit on the bound for the stability of matter. These efforts have culminated in the work of Lieb and Thirring,^{15,16} whose result for q species of fermions (units: $2m = e = h = 1$) moving in the field of M nuclei with positive charges Z_j is as follows:

$$E_{\min} \geq -1.31 q^{2/3} N \left[1 + \left(\sum_{j=1}^M Z_j^{7/3} / N \right)^{1/2} \right]^2.$$

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Summation of partial wave expansions in the scattering by long range potentials. I ^{a)}

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Punctual Padé approximants are considered as a summation method of the slowly convergent partial wave expansions associated with the scattering by long range potentials. The asymptotic behavior of the family of sequences $[n, n+m]$, with fixed n , of the Padé table, is studied. A set of theorems are proven, which show that their rate of convergence increases rapidly with n . It is noted that these approximants may be computed by means of the recurrent ϵ and η algorithms.

1. INTRODUCTION

On the calculation of nonrelativistic scattering amplitudes, three significant energy ranges may be separated. The limits of these regions are not well defined and depend on the particular process and interaction considered. In the low energy range, calculations may be performed in a satisfactory way by means of the partial wave method, using a small number of phase shifts. In the high energy region, the first term of the Born series is able to give good results. Problems arise when calculating in the so-called intermediate energy range. When extending the first method to this region, the number of phase shifts, required to get a good approximation for the scattering amplitude, increases with the energy. Otherwise, when using the Born series, an increasing number of perturbative terms are necessary as the energy decreases. In other words, the rate of convergence of both expansions is slow, and calculations become very involved in the intermediate energy region. Depending on the process considered, other methods of calculation, such as the distorted wave or semiclassical approximation, are rather efficient in that energy range. However, an interesting global approach is to keep the original perturbative or partial wave expansions, and to find adequate mathematical summation methods, in order to avoid the calculation of high order terms in the series.

For the perturbative series, the Padé approximants have been proposed as a proper method to obtain significant values for the scattering amplitude, when the expansion is slowly convergent or divergent. Formal properties of the convergence of these approximants have been studied,¹ and different applications show that they are able to extend the information contained in the low-order terms of the Born series, for medium energies² even outside of the convergence disk of the original perturbative series.

In atomic and molecular collision physics, the interactions are mainly governed by long range potentials. This determines the requirement of calculating several hundreds, or even thousands, of phase shifts, in order to get accurate values for the angular distributions in the intermediate energy region, when using the partial

wave expansion.³ Then, it is very important to find a method to efficiently summate this type of series. With this scope, some efforts have been made before by using the Padé—Legendre approximants.⁴ However, no convergence theorems are available yet for these algorithms, and they do not seem to be readily computable up to the large orders required in atomic and molecular collision calculations. Other approaches,⁵ for which formal convergence properties are known, require solving systems of nonlinear equations, which become very involved.

Punctual Padé approximants are considered in this work, as a summation method of partial wave expansions. We prove a set of theorems regarding their asymptotic rate of convergence, when long range potentials are present, showing it to be greater than that of the original expansions. In Sec. 2 the approximants are introduced, and we show that they may be used, in principle, to summate any formal series. Furthermore, they can be obtained recurrently, allowing for a simple calculation of the high order ones. In Sec. 3 asymptotic estimates are obtained for the sequence of partial wave sums of the scattering amplitude and total cross section, for long range potentials. By using them, in Sec. 4, three theorems are proved from which the main results are established.

2. PUNCTUAL PADÉ APPROXIMANTS

The $[N, M]_{C(z)}$ Padé approximant to a formal power series

$$C(z) = \sum_{r=0}^{\infty} b_r z^r \quad (2.1)$$

is defined as a rational function¹

$$[N, M]_{C(z)} = \frac{a_0 + a_1 z + \dots + a_M z^M}{1 + b_1 z + \dots + b_N z^N} \quad (2.2)$$

which is determined by requiring that its McLaurin expansion agree with that of $C(z)$ through the power z^{N+M} , that is,

$$C(z) - [N, M]_{C(z)} = O(z^{N+M+1}), \quad (2.3)$$

A special case of (2.1) is the infinite sum

$$C(1) = \sum_{r=0}^{\infty} b_r \quad (2.4)$$

with partial sums

$$C_m = \sum_{r=0}^m b_r. \quad (2.5)$$

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The Padé approach can be used, in principle, to evaluate either the sum $C(1)$, or the limiting value of the sequence $\{C_m\}$, by defining, formally, the punctual Padé approximants (we shall refer to them as PPA), by Eq. (2.3) and setting $z=1$ in Eq. (2.2). It is clear, however, that whether this approximation scheme proves to be of advantage or not, will depend, in general, on the particular series or sequences considered. The approximations so defined, determine a doubly infinite array of rational functions, from which many sequences may be selected. Of particular interest, are the $[n, n+m]_{C(1)}$ approximants, with $m \geq 0$. They coincide with the n th order transforms $E_n(C_m)$ of the sequence C_m , first considered by Shanks⁶ in his thesis, which were introduced as formal generalizations of Aitken's extrapolation formula, in searching for means of transforming divergent or slowly convergent sequences. These transformations are nonlinear, and are given by the determinantal quotients⁶

$$E_n(C_m) = [n, n+m]_{C(1)} = \frac{H_n^{(m)}\{C_r\}}{H_n^{(m)}\{\Delta^2 C_r\}}, \quad m, n \geq 0, \quad (2.6)$$

or, equivalently⁷

$$[n, n+m]_{C(1)} = \frac{H_n^{(0)}\{\Delta^r C_m\}}{H_n^{(2)}\{\Delta^r C_m\}}, \quad m, n \geq 0, \quad (2.7)$$

where for $r \geq 1$, $\Delta^r C_m = \Delta^{r-1} C_{m+1} - \Delta^{r-1} C_m$, $\Delta^0 C_m = C_m$, and we have used the Hankel determinants defined, for a given sequence $\{f_r\}$, by

$$H_n^{(m)}\{f_r\} = \begin{vmatrix} f_m & f_{m+1} & \cdots & f_{m+k-1} \\ f_{m+1} & f_{m+2} & \cdots & f_{m+k} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ f_{m+k-1} & f_{m+k} & \cdots & f_{m+2k-2} \end{vmatrix}.$$

For large n , owing to the numerical difficulties involved, the $[n, n+m]_{C(1)}$ approximants are not readily computable from Eqs. (2.6) and (2.7). By appealing to a classical, but little known determinant identity, Wynn found a recurrent method for calculating these transformations.⁸ This resulted in the epsilon algorithm, of which Bauer's eta algorithm is a more stable variant,⁹ from the numerical point of view. In this way, one has an efficient manner of generating the PPA while being able, at the same time, to check the convergence pattern of successive approximations.

It is worthwhile to state some interesting properties of these approximations which may be easily deduced from Eq. (2.6). Firstly, let us note that

$$E_n(C_m) = p_1 C_m + p_2 C_{m+1} + \cdots + p_{n+1} C_{m+n}$$

with $p_1 + p_2 + \cdots + p_{n+1} = 1$, which allows us to view the $E_n(C_m)$ transformation as a weighted average of $C_m, C_{m+1}, \dots, C_{m+n}$. It is, however, a nonlinear average, since the p_i are functions of the C_r . Secondly, if the sequence of interest is

$$C_m = A + KC'_m$$

with A and K constants, then

$$E_n(C_m) = A + KE_n(C'_m). \quad (2.8)$$

This relation is very useful, as will be seen, when proving formal properties of the $E_n(C_m)$.

Furthermore, it is clear that the PPA $[n, n+m]_{C(1)}$ may be seen, equivalently, as a nonlinear transformation of the sequence $\{C_m\}$ (given $C_m, C_{m+1}, \dots, C_{m+2n}$), or of the series $C(1)$ (given $b_0, b_1, \dots, b_{m+2n}$). Because of this equivalence, reference will be made, alternatively, to the sequence or to the series, and in order to keep the well established notation for Padé approximants, we shall define

$$[n, n+m]_{\{C_r\}} \equiv [n, n+m]_{C(1)}.$$

3. THE SEQUENCE OF PARTIAL WAVE SUMS

A. The scattering amplitude

The partial wave expansion of the scattering amplitude in terms of the phase shifts δ_l , is given by

$$\begin{aligned} f(\theta) &= \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) [\exp(2i\delta_l) - 1] P_l(\cos\theta) \\ &= \sum_{l=0}^{\infty} a_l P_l(\cos\theta), \end{aligned} \quad (3.1)$$

where k is the magnitude of the wave vector, and the $\{P_l\}$ are the Legendre polynomials.

Our concern in this work will be to deal with potentials having a long range behavior

$$U(r) \sim \frac{c}{r^{\alpha+2}}, \quad \alpha \geq 0, \quad (3.2)$$

where α is an integer. In this way, we shall include in our treatment usual potentials present in atomic and molecular collision processes, which determine a slow convergence of expansion (3.1) (i. e., $\alpha = 0, 2, 4$, which corresponds respectively, to the charge dipole, induced polarization, and Van der Waals interactions.¹⁰ The convergence of series (3.1) is governed, in these cases, by the high order phase shifts, which in turn, are mainly related to the long range tail of the potentials. In order to have the convergence properties of the sequence of partial sums of expansion (3.1) explicitly dependent on the latter, we shall define them in the following way,

$$\begin{aligned} f_m(\theta) &= \sum_{l=0}^m a_l P_l(\cos\theta) \\ &= f(\theta) - \sum_{l=m+1}^{\infty} a_l P_l(\cos\theta). \end{aligned} \quad (3.3)$$

The last equality holds when series (3.1) is convergent. For potentials of the type given by Eq. (3.2), this requires $\alpha \geq 0$ for $-1 < \cos\theta < 1$, while for $\cos\theta = \pm 1$, the restrictions, are, respectively, $\alpha \geq 2$, and $\alpha \geq 1$.

In what follows, asymptotic expressions for the phase shifts will be obtained. By using them, we shall be able to get estimates for $f_m(\theta)$ valid for $m \rightarrow \infty$.

In general, we shall say that A_m asymptotically approaches B_m , that is

$$A_m \sim B_m$$

if given a small positive quantity ϵ , an integer m_0 can be found such that, for $m \geq m_0$

$$\frac{|A_m - B_m|}{|A_m|} < \epsilon.$$

It is well known that the δ_i are given asymptotically in l , by the semiclassical formula¹¹

$$\delta_l \sim \int_{r_1}^{\infty} dr F_1(r) - \int_{r_0}^{\infty} dr F_0(r). \quad (3.4)$$

In this equation $F_1(r) = [k^2 - U(r) - L^2/r^2]^{1/2}$, $F_0(r) = (k^2 - L^2/r^2)^{1/2}$, $U(r) = (2\mu/\hbar^2)V(r)$, $L = l + \frac{1}{2}$, μ is the reduced mass of the system, $V(r)$ the interaction potential, r_1 the outermost zero of $F_1(r)$, and r_0 the positive root of $F_0(r)$. For potentials of the type (3.2), let us take account of the fact that for $l \gg 1$, one has $r_1 \approx r_0 = L/k \gg 1$. Then, one can replace the estimate given by Eq. (3.2) for $U(r)$ in Eq. (3.4), and expand δ_l in an asymptotic series

$$\begin{aligned} \delta_l &\sim -\frac{1}{2} \int_{r_0}^{\infty} \frac{U(r)dr}{F_0(r)} - \frac{1}{8} \int_{r_0}^{\infty} \frac{U^2(r)dr}{F_0^3(r)} + \dots \\ &= -\frac{c}{2k} \frac{1}{r_0^{\alpha+1}} \int_0^{\pi/2} d\theta (\sin\theta)^\alpha - \frac{c^3}{8k^3} \frac{1}{r_0^{2\alpha+3}} \int_0^{\pi/2} d\theta \\ &\quad \times \frac{(\sin\theta)^{2\alpha+2}}{(\cos\theta)^2} + \dots \end{aligned} \quad (3.5)$$

Performing the integrals in Eq. (3.5), we get

$$\delta_l \sim \frac{-ck^\alpha}{2(l + \frac{1}{2})^{\alpha+1}} I_\alpha + O\left(\frac{k^\alpha}{(l + \frac{1}{2})^{2\alpha+3}}\right), \quad (3.6)$$

where

$$I_\alpha = \begin{cases} \pi/2 & \text{for } \alpha=0, \\ \frac{(\alpha-1)!!}{\alpha!!} \frac{\pi}{2}, & \text{for even } \alpha > 0, \\ \frac{(\alpha-1)!!}{\alpha!!} & \text{for odd } \alpha. \end{cases}$$

It should be remarked that the first term in Eq. (3.6) coincides with the Massey-Mohr approximation¹² for the phase shifts.

Using the fact that the $\delta_i \rightarrow 0$ for $l \rightarrow \infty$, we may expand $\exp(2i\delta_l)$ in powers of δ_l in each term of the series in Eq. (3.3), in order to get an asymptotic expression of $f_m(\theta)$ for large m ,

$$\begin{aligned} f_m(\theta) &= f(\theta) - \frac{2}{k} \sum_{l=m+1}^{\infty} \{ (l + \frac{1}{2})\delta_l + O[(l + \frac{1}{2})\delta_l^2] \} P_l(\cos\theta) \\ &\sim f(\theta) + K \sum_{l=m+1}^{\infty} \left[\frac{1}{(l + \frac{1}{2})^\alpha} + O\left(\frac{1}{(l + \frac{1}{2})^{2\alpha+1}}\right) \right] P_l(\cos\theta), \end{aligned} \quad (3.7)$$

where $K = ck^{\alpha-1}I_\alpha$, and we have used Eq. (3.6) for the phase shifts. By defining

$$S_m(\theta) = S_m^{0,\alpha}(\theta) = \sum_{l=m+1}^{\infty} \frac{P_l(\cos\theta)}{(l + \frac{1}{2})^\alpha} \quad (3.8)$$

we write the asymptotic estimate for $f_m(\theta)$ as

$$f_m(\theta) \sim f(\theta) + KS_m(\theta). \quad (3.9)$$

B. Asymptotic estimates of $S_m(\theta)$

In what follows, we shall obtain the explicit dependence on m of the asymptotic sequence $\{S_m^{0,\alpha}(\theta)\}$.

Lemma 3.1: The sequence $S_m^{0,\alpha}(\theta)$ defined by Eq. (3.8) has the following asymptotic behavior (α integer):

$$S_m^{0,\alpha}(\theta) \sim \frac{\sin(m'\theta - \pi/4)}{(2\pi \sin\theta \sin^2\theta/2)^{1/2}} \cdot \frac{1}{M^{\alpha+1/2}} \quad (0 < \theta < \pi, \alpha \geq 0), \quad (3.10a)$$

$$S_m^{0,\alpha}(0) \sim \frac{-1}{(1-\alpha)M^{\alpha-1}} \quad (\alpha \geq 2), \quad (3.10b)$$

$$S_m^{0,\alpha}(\pi) \sim \frac{(-1)^{m+1}}{2M^\alpha} \quad (\alpha \geq 1), \quad (3.10c)$$

where $M = m + \frac{1}{2}$ and $m' = m + 1$.

Proof: We use the Euler-McLaurin summation formula,¹³ which for our case can be written

$$\begin{aligned} S_m^{0,\alpha}(\theta) &= \int_m^\infty \frac{P_l(\cos\theta)}{(l + \frac{1}{2})^\alpha} dl - \frac{P_m(\cos\theta)}{2M^\alpha} \\ &\quad - \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} \frac{d^{2n-1}}{dl^{2n-1}} \left(\frac{P_l(\cos\theta)}{(l + \frac{1}{2})^\alpha} \right)_{l=m}, \end{aligned} \quad (3.11)$$

where the B_{2n} are the Bernoulli numbers.

Let us first consider $0 < \theta < \pi$. In this case the following asymptotic expansion holds,¹⁴

$$P_l(\cos\theta) \sim \left(\frac{2}{\pi \sin\theta} \right)^{1/2} \frac{\cos\Omega_L}{L^{1/2}} + O\left(\frac{1}{L^{3/2}}\right), \quad (3.12)$$

where, as before, $L = l + \frac{1}{2}$, and $\Omega_L = L\theta - \pi/4$. By using the fact that for $n \geq 1$,

$$\begin{aligned} \int_A^\infty \frac{\cos x}{x^{n/2}} dx &\rightarrow \frac{\sin A}{A^{n/2}} + O\left(\frac{1}{A^{n/2+1}}\right), \\ \int_A^\infty \frac{\cos x}{x^{n/2}} dx &\rightarrow \frac{\cos A}{A^{n/2}} + O\left(\frac{1}{A^{n/2+1}}\right), \end{aligned}$$

and the expression (3.12) we can show that

$$\int_m^\infty \frac{P_l(\cos\theta)}{(l + \frac{1}{2})^\alpha} dl \sim -\frac{a}{M^{\alpha+1/2}} \sin\Omega_M + O\left(\frac{1}{M^{\alpha+3/2}}\right) \quad (3.13)$$

with $a = (2/\pi \sin\theta)^{1/2}$. Furthermore, by a straightforward calculation

$$\begin{aligned} &\sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} \frac{d^{2n-1}}{dl^{2n-1}} \left[\frac{P_l(\cos\theta)}{(l + \frac{1}{2})^\alpha} \right]_{l=m} \\ &\sim \frac{a}{M^{\alpha+1/2}} \sin\Omega_M \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} (-1)^n \theta^{2n} + O\left(\frac{1}{M^{\alpha+3/2}}\right) \\ &= \frac{a}{M^{\alpha+1/2}} \sin\Omega_M \left(\frac{\theta}{2} \cot \frac{\theta}{2} - 1 \right) + O\left(\frac{1}{M^{\alpha+3/2}}\right). \end{aligned} \quad (3.14)$$

Finally, replacing Eqs. (3.12), (3.13), and (3.14) in (3.11), we get

$$S_m^{0,\alpha}(\theta) \sim A(\theta) \frac{\sin(m'\theta - \pi/4)}{M^{\alpha+1/2}} + O\left(\frac{1}{M^{\alpha+3/2}}\right),$$

where $A(\theta) = -(2\pi \sin\theta \sin^2\theta/2)^{-1/2}$, from which Eq. (3.10a) follows.

Let us consider now the particular cases $\theta = 0$ and $\theta = \pi$, for which the $P_l(\cos\theta)$ take the simple values 1 and $\cos\pi l$, respectively.

For $\theta = 0$ we will have:

$$\begin{aligned} \int_m^\infty \frac{dl}{(l + \frac{1}{2})^\alpha} &= \frac{-1}{(1-\alpha)M^{\alpha-1}}, \\ \sum_{n=1}^{\infty} \frac{B_{2n}}{(2n)!} \frac{d^{2n-1}}{dl^{2n-1}} \left[\frac{1}{(l + \frac{1}{2})^\alpha} \right]_{l=m} &\sim -\frac{\alpha B_2}{2M^{\alpha+1}} + O\left(\frac{1}{M^{\alpha+2}}\right), \end{aligned}$$

replacing again in Eq. (3.11), we immediately obtain Eq. (3.10b). We note that we must require $\alpha > 1$, to have bounded quantities.

For $\theta = \pi$, replacing the asymptotic estimates

$$\begin{aligned} \int_m^\infty \frac{\cos \pi l}{(l + \frac{1}{2})^\alpha} dl &\sim \frac{(-1)^m \alpha}{\pi^2 M^{\alpha+1}} + O\left(\frac{1}{M^{\alpha+3}}\right) \\ \sum_{n=1}^\infty \frac{B_{2n}}{(2n)!} \frac{d^{2n-1}}{dl^{2n-1}} \left[\frac{\cos \pi l}{(l + \frac{1}{2})^\alpha} \right]_{l=m} &\sim \frac{(-1)^m \alpha}{M^{\alpha+1}} \sum_{n=1}^\infty \frac{B_{2n}}{(2n)!} (-1)^n (2n-1) \pi^{2n-2} + O\left(\frac{1}{M^{\alpha+2}}\right) \\ &= \frac{(-1)^m \alpha}{M^{\alpha+1}} \left(\frac{1}{\pi^2} - \frac{1}{4} \right) + O\left(\frac{1}{M^{\alpha+2}}\right), \end{aligned}$$

in Eq. (3.12), we obtain the statement given by Eq. (3.10c). In this case our calculation requires $\alpha > 0$.

It should be remarked that our restrictions on the value of α are the usual ones to assure the convergence of the partial wave expansion, and, consequently, the validity of Eq. (3.3).

We shall now derive a second lemma, that will be used in the proof of the theorems in the next section. We first define the quantities $S_m^{r+1, \alpha}$ by the recurrent relation ($r \geq 0$)

$$S_m^{r+1, \alpha}(\theta) = S_{m+1}^{r, \alpha}(\theta) + S_{m-1}^{r, \alpha}(\theta) - 2 \cos \theta S_m^{r, \alpha}(\theta). \quad (3.15)$$

Then, we show in Appendix A that

$$\begin{aligned} S_m^{r+1, \alpha}(\theta) &= -(\alpha + \frac{1}{2}) \sum_{n=1}^\infty \frac{(\alpha + n - 1)!}{n! \alpha!} \\ &\quad \times [S_{m+1}^{r, \alpha+n}(\theta) + (-1)^n S_{m-1}^{r, \alpha+n}(\theta)]. \end{aligned} \quad (3.16)$$

Lemma 3.2: The sequence $\{S_m^{r, \alpha}(\theta)\}$ has, for $0 < \theta < \pi$, the following asymptotic behavior ($r, \alpha \geq 0$):

$$\begin{aligned} S_m^{r, \alpha}(\theta) &\sim -\frac{(2\alpha + 2r - 1)!! \sin^r \theta}{[2\pi \sin^2(\theta/2) \sin \theta]^{1/2} (2\alpha - 1)!! M^{\alpha+r+1/2}} \\ &\quad \times \sin\left(m'\theta - \frac{\pi}{4} - r\frac{\pi}{2}\right) + O\left(\frac{1}{M^{\alpha+r+3/2}}\right). \end{aligned} \quad (3.17)$$

Proof: We write Eq. (3.16) for $r=0$,

$$S_m^{1, \alpha} = -(\alpha + \frac{1}{2}) \sum_{n=1}^\infty \frac{(\alpha + n - 1)!}{n! \alpha!} [S_{m+1}^{0, \alpha+n} + (-1)^n S_{m-1}^{0, \alpha+n}].$$

Then from Eq. (3.10a)

$$\begin{aligned} S_m^{1, \alpha}(\theta) &\sim -(\alpha + \frac{1}{2}) [S_{m+1}^{0, \alpha+1} - S_{m-1}^{0, \alpha+1}] \\ &\quad \sim \frac{A(\theta)(\alpha + \frac{1}{2})}{M^{\alpha+3/2}} 2 \sin \theta \sin\left(m'\theta - \frac{\pi}{4} - \frac{\pi}{2}\right) + O\left(\frac{1}{M^{\alpha+5/2}}\right). \end{aligned}$$

By successive application of this procedure we arrive at Eq. (3.17).

C. The total cross section

In terms of the phase shifts the total differential cross section is given by the expansion

$$Q = \frac{4\pi}{k^2} \sum_{l=0}^\infty (2l+1) \sin^2 \delta_l, \quad (3.18)$$

and we may define the sequence of partial sums in the form

$$\begin{aligned} Q_m &= \frac{4\pi}{k^2} \sum_{l=0}^m (2l+1) \sin^2 \delta_l \\ &= Q - \frac{4\pi}{k^2} \sum_{l=m+1}^\infty (2l+1) \sin^2 \delta_l. \end{aligned} \quad (3.19)$$

The last equality holds when the series (3.18) is convergent. For potentials of the type (3.2) this requires $\alpha > 0$ [cf. Eq. (3.6)], and in this case we may expand $\sin \delta_l$ in powers of δ_l and use Eq. (3.6), to obtain an asymptotic expression for Q_m ,

$$\begin{aligned} Q_m &\sim Q - \frac{8\pi}{k^2} \sum_{l=m+1}^\infty (l + \frac{1}{2}) \delta_l^2 \\ &\sim Q - K' \sum_{l=m+1}^\infty (l + \frac{1}{2})^{-2\alpha-1} \end{aligned} \quad (3.20)$$

with $K' = 2\pi c^2 k^{2\alpha-2} l_\alpha^2$.

By now using the Euler–McLaurin formula to summate the series in Eq. (3.20), we get an asymptotic estimate for Q_m ,

$$Q_m \sim Q + \frac{K'}{2\alpha} \frac{1}{M^{2\alpha}} + O\left(\frac{1}{M^{2\alpha+1}}\right). \quad (3.21)$$

We note that Eq. (3.21) shows similar asymptotic behavior for Q_m and $f_m(0)$ [cf. Eqs. (3.9) and (3.10b)], that is, both sequences tend towards their limits in a monotonous way, dependent on a power of M^{-1} . By recalling the optical theorem, Eq. (3.21) gives the behavior of $\text{Im} f_m(0)$, while that of the $\text{Re} f_m(0)$ is given by Eqs. (3.10b) and (3.9).

4. ASYMPTOTIC BEHAVIOR OF THE PPA TO THE PARTIAL WAVE EXPANSIONS OF $f(\theta)$ AND Q

Theorem 4.1: For θ such that $0 < \theta < \pi$, and for fixed n , the PPA $[n, n+m]$ to the sequence

$$S_m(\theta) = \sum_{l=m+1}^\infty P_l(\cos \theta) / (l + \frac{1}{2})^\alpha, \quad (\alpha \geq 0)$$

has the following asymptotic behavior

$$\begin{aligned} [n, n+m]_{\{S_m(\theta)\}} &\sim [(-1)^{N+1} (\sin \theta)^{2(n-N)-1/2} 2^{N-2n} (2\alpha + 2N - 1)!! N! \\ &\quad (\sin \Lambda_{m+n})^{2(2N-n)+1} / [(2\pi)^{1/2} (2\alpha - 1)!! \\ &\quad (\sin \theta/2)^{2n+1} M^{\alpha+2N+1/2}] \end{aligned} \quad (4.1)$$

where $N = n/2$, for even n , $N = (n-1)/2$ for odd n , and $\Lambda_j = (j+1)\theta - \pi/4$.

Proof: We use definition Eq. (2.6) for the $[n, n+m]$ approximant and we first consider the numerator $H_{n+1}^{(m)} \{S_r\}$. We add by pairs its successive even (and odd) order columns, and rows, using Eq. (3.15), in the following generic way,

$$\begin{aligned} \begin{vmatrix} S_m^{i, \alpha} & S_{m+1}^{i, \alpha} & S_{m+2}^{i, \alpha} \\ S_{m+1}^{i, \alpha} & S_{m+2}^{i, \alpha} & S_{m+3}^{i, \alpha} \\ S_{m+2}^{i, \alpha} & S_{m+3}^{i, \alpha} & S_{m+4}^{i, \alpha} \end{vmatrix} &= \begin{vmatrix} S_m^{i, \alpha} & S_{m+1}^{i, \alpha} & 2 \cos \theta S_{m+1}^{i, \alpha} + S_{m+1}^{i+1, \alpha} \\ S_{m+1}^{i, \alpha} & S_{m+2}^{i, \alpha} & 2 \cos \theta S_{m+2}^{i, \alpha} + S_{m+2}^{i+1, \alpha} \\ S_{m+2}^{i, \alpha} & S_{m+3}^{i, \alpha} & 2 \cos \theta S_{m+3}^{i, \alpha} + S_{m+3}^{i+1, \alpha} \end{vmatrix} \\ &= \begin{vmatrix} S_m^{i, \alpha} & S_{m+1}^{i, \alpha} & S_{m+1}^{i+1, \alpha} \\ S_{m+1}^{i, \alpha} & S_{m+2}^{i, \alpha} & S_{m+2}^{i+1, \alpha} \\ S_{m+2}^{i, \alpha} & S_{m+3}^{i, \alpha} & S_{m+3}^{i+1, \alpha} \end{vmatrix}. \end{aligned}$$

By repeated application of the procedure, we obtain

$$H_{n+1}^{(m)}\{S_r\} = \begin{vmatrix} S_m^{0,\alpha} & S_{m+1}^{0,\alpha} & S_{m+1}^{1,\alpha} & S_{m+2}^{1,\alpha} & \dots & S_{m+n-N}^{N,\alpha} \\ S_{m+1}^{0,\alpha} & S_{m+2}^{0,\alpha} & S_{m+2}^{1,\alpha} & S_{m+3}^{1,\alpha} & \dots & S_{m+n-N+1}^{N,\alpha} \\ S_{m+1}^{1,\alpha} & S_{m+2}^{1,\alpha} & S_{m+2}^{2,\alpha} & S_{m+3}^{2,\alpha} & \dots & S_{m+n-N+1}^{N+1,\alpha} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ S_{m+n-N}^{N,\alpha} & S_{m+n-N+1}^{N,\alpha} & S_{m+n-N+1}^{N+1,\alpha} & S_{m+n-N+2}^{N+1,\alpha} & \dots & S_{m+2n-2N}^{2N,\alpha} \end{vmatrix} \\ = D_{n+1}^m \{S_{m+k}^{j,\alpha}\}, \quad (4.2)$$

where N is defined as above. We shall now perform an asymptotic estimate of $D_{n+1}^m \{S_{m+k}^{j,\alpha}\}$, by considering $m \rightarrow \infty$ with fixed n , and retaining only the lowest powers of $M^{-1/2}$ in the calculations. In this way, from Eq. (3.17), we have

$$S_{m+k}^{j,\alpha} \sim A(\theta) \frac{(2\alpha + 2j - 1)!! (\sin\theta)^j}{(2\alpha - 1)!! M^{\alpha+j+1/2}} \\ \times \sin(\Lambda_{m+k} - j\pi/2), \quad \alpha \geq 0 \\ = h_j \sin(\Lambda_{m+k} - j\pi/2) \quad (4.3)$$

with $\Lambda_{m+k} = (m+k+1)\theta - \pi/4$, as above. Then, using Eq. (4.3) in Eq. (4.2)

$$H_{n+1}^{(m)}\{S_r\} \sim D_{n+1}^m \{h_j \sin(\Lambda_{m+k} - j\pi/2)\} \\ = (-1)^{(N+1)(n-2N)} (\sin\theta)^{2(n-N)} \\ \times (\sin\Lambda_{m+n})^{2N-n+1} H_{N+1}^{(0)}\{h_r\} H_{n-N}^{(0)}\{h_r\} \quad (4.4)$$

with

$$H_j^{(0)}\{h_r\} = \frac{(\sqrt{2} \sin\theta)^j (A(\theta))^j}{[(2\alpha - 1)!!]^{j-1} M^{j(\alpha+j-1/2)}} \\ \times \prod_{p=1}^{j-1} (2\alpha + 2p - 1)!! p!. \quad (4.5)$$

The last equality in Eq. (4.4) and the result given by Eq. (4.5) follow from algebraic calculations described in Appendix B, sections 1 and 2, respectively.

In order to estimate the asymptotic behavior of the denominator $H_n^{(m)}\{\Delta^2 S_r\}$ in Eq. (2.6), we note that

$$\Delta^2 S_r = \Delta(S_{r+1} - S_r) = S_{r+2} - 2S_{r+1} + S_r \\ = 2(\cos\theta - 1)S_{r+1} + S_{r+1}^{1,\alpha},$$

where Eq. (3.15) for $r=0$, has been used in the last step. Then,

$$H_n^{(m)}\{\Delta^2 S_r\} = H_n^{(m)}\{2(\cos\theta - 1)S_{r+1} + S_{r+1}^{1,\alpha}\} \\ \sim (-1)^n [2 \sin\theta/2]^{2n} H_n^{(m+1)}\{S_r\} \quad (4.6)$$

and it is seen that this determinant can also be evaluated asymptotically, by using Eq. (4.4). Replacing the estimates obtained for the numerator and denominator in Eq. (2.6), we get

$$[n, n+m]_{\{S_m^{(0)}\}} \sim \frac{(-1)^N (\sin\theta)^{2(n-2N)} H_{N+1}^{(0)}\{h_r\}}{(2 \sin\theta/2)^{2n} H_N^{(0)}\{h_r\}} \\ \times (\sin\Lambda_{m+n})^{2(2N-n)+1} \quad (4.7)$$

and using Eq. (4.5) in Eq. (4.7), Eq. (4.1) follows.

We note that for some particular values of $m+n$, and a given θ , $\sin\Lambda_{m+n} = 0$, and consequently Eq. (4.1)

will predict $[n, n+m] \sim 0$ (even n) or $[n, n+m] \sim \infty$ (odd n). Actually, we have arrived at Eq. (4.1) by using the estimate given by Eq. (4.3) which results from keeping only the leading term in an asymptotic series for $S_{m+k}^{j,\alpha}$, in powers of $M^{-1/2}$. Including the higher orders, the precision of the $[n, n+m]$ for these isolated cases would be slightly better in the first case, and slightly poorer in the second, than that given generally by Eq. (4.1), without the oscillating factor $\sin\Lambda_{m+n}$.

Theorem 4.2: The PPA $[n, n+m]$ to the sequence

$$S_m(0) = \sum_{l=m+1}^{\infty} \frac{1}{(l + \frac{1}{2})^\alpha}, \quad \alpha \geq 2$$

has, for fixed n , the following asymptotic behavior

$$[n, n+m]_{\{S_m^{(0)}\}} \sim \frac{(\alpha - 2)! n!}{(n + \alpha - 1)! M^{\alpha-1}}. \quad (4.8)$$

Proof: We start with the asymptotic estimate for $S_m(0)$, given by Eq. (3.10b),

$$S_m(0) \sim \frac{1}{(\alpha - 1) M^{\alpha-1}} \quad (\alpha \geq 2),$$

to obtain

$$\Delta^r S_m \sim \frac{(-1)^r (\alpha + r - 2)!}{(\alpha - 1)! M^{\alpha+r-1}} \quad (r \geq 0). \quad (4.9)$$

Using this relation in the Hankel determinants in Eq. (2.7), we obtain (Appendix B 3)

$$H_{n+1}^{(0)}\{\Delta^r S_m\} \sim \frac{H_n^{(\alpha-2)}\{r!\}}{[(\alpha - 1)!]^{n+1} M^{(n+\alpha-1)(n+1)}}. \quad (4.10a)$$

In the same way,

$$H_n^{(2)}\{\Delta^r S_m\} \sim \frac{H_n^{(\alpha)}\{r!\}}{[(\alpha - 1)!]^n M^{n(n+\alpha)}} \quad (4.10b)$$

with (Appendix B 2)

$$H_{n+1}^{(m)}\{r!\} = \prod_{p=0}^n (m+p)! p! \quad (4.11)$$

Finally, we obtain

$$[n, n+m]_{\{S_m^{(0)}\}} = \frac{H_{n+1}^{(0)}\{\Delta^r S_m\}}{H_n^{(2)}\{\Delta^r S_m\}} \\ \sim \frac{H_n^{(\alpha-2)}\{r!\}}{(\alpha - 1)! H_n^{(\alpha)}\{r!\} M^{\alpha-1}}. \quad (4.12)$$

Using Eq. (4.11), our statement in Eq. (4.8) follows.

Theorem 4.3: The PPA $[n, n+m]$, to the sequence

$$S_m(\pi) = \sum_{l=m+1}^{\infty} \frac{(-1)^l}{(l + \frac{1}{2})^\alpha}, \quad \alpha \geq 1$$

has, for fixed n , the following asymptotic behavior,

$$[n, n+m]_{\{S_m^{(\pi)}\}} \sim \frac{(-1)^{m+1} (\alpha + n - 1)! n!}{2^{2n+1} (\alpha - 1)! M^{\alpha+2n}}. \quad (4.13)$$

Proof: We first consider the asymptotic estimate of $S_m(\pi)$ given by Eq. (3.10c),

$$S_m(\pi) \sim \frac{(-1)^{m+1}}{2M^\alpha}, \quad \alpha \geq 1,$$

and we get, using Eq. (4.9)

$$\Delta^r [(-1)^m S_m(\pi)] \sim \frac{(-1)^{r+1} (\alpha + r - 1)!}{2(\alpha - 1)! M^{\alpha+r}}. \quad (4.14)$$

We can now use the the property

$$H_n^{(m)}\{S_r\} = (-1)^{nm} H_n^{(m)}\{(-1)^r S_r\} \\ = (-1)^{nm} H_n^{(0)}\{\Delta^r [(-1)^m S_m]\}$$

and Eq. (4.6), to write

$$H_n^{(m)}\{\Delta^2 S_r\} \sim (-1)^n 2^{2n} H_n^{(m+1)}\{S_r\} \\ = (-1)^n 2^{2n} (-1)^{n(m+1)} H_n^{(m+1)}\{(-1)^r S_r\} \\ = (-1)^{nm} 2^{2n} H_n^{(0)}\{\Delta^r [(-1)^{m+1} S_{m+1}]\} \quad (4.15)$$

By comparison of Eqs. (4.14) and (4.9), and the use of Eqs. (4.10a) and (4.15), we get [cf. Eq. (2.6)]

$$[n, n+m]_{\{S_m(\alpha)\}} = \frac{H_n^{(m)}\{S_r\}}{H_n^{(m)}\{\Delta^2 S_r\}} \\ \sim \frac{(-1)^{m+1}}{2^{2n+1}(\alpha-1)! M^{\alpha+2n}} \cdot \frac{H_n^{(\alpha-1)}\{r!\}}{H_n^{(\alpha-1)}\{r!\}}.$$

Using the Hankel determinant given by Eq. (4.1) we obtain Eq. (4.13)

It should be remarked, that Theorems 4.2 and 4.3 can be viewed as generalizations of Theorems 11 and 13 by Wynn,⁷ which correspond, respectively, to the particular cases $\alpha=2$ and $\alpha=1$.

Corollary 4.1: The PPA $[n, n+m]$ to the partial wave expansion of the scattering amplitude $f(\theta)$, corresponding to a central potential with a long range tail of the type given by Eq. (3.2)

$$U(r)_{r \rightarrow \infty} \sim \frac{c}{r^{\alpha+2}} \quad (4.16)$$

has, for fixed n , the asymptotic behavior

$$[n, n+m]_{f(0)} \sim f(0) + \frac{K(\alpha-2)! n!}{(n+\alpha-1)! M^{\alpha-1}} \quad (\alpha \geq 2), \quad (4.17a)$$

$$[n, n+m]_{f(\theta)} \sim f(\theta) + [(-1)^{N+1} K(\sin\theta)^{2(n-N)-1} / 2^{2N-2n} \\ \times (2\alpha+2N-1)!! N! (\sin\Lambda_{m+n})^{2(2N-n)+1} / \\ [(2\pi)^{1/2} (2\alpha-1)!! (\sin\theta/2)^{2n+1} \\ \times M^{\alpha+2N+1/2}] \quad (\alpha \geq 0, 0 < \theta < \pi) \quad (4.17b)$$

$$[n, n+m]_{f(\pi)} \sim f(\pi) + \frac{(-1)^{m+1} K(\alpha+n-1)! n!}{2^{2n+1}(\alpha-1)! M^{\alpha+2n}} \quad (\alpha \geq 1), \quad (4.17c)$$

where $K = ck^{\alpha-1} I_\alpha$, $\Lambda_j = (j+1)\theta - \pi/4$, $M = m + \frac{1}{2}$, $N = n/2$ for even n , and $N = (n-1)/2$, for odd n .

This corollary follows from the asymptotic relation between $f_m(\theta)$ and $S_m(\theta)$ [cf. Eq. (3.9)], the property of the PPA showed in Eq. (2.8), and the results of theorems 4.1, 4.2, and 4.3.

Corollary 4.2: The PPA $[n, n+m]$ to the partial wave expansion of the total cross section Q corresponding to a central potential with the behavior of Eq. (4.16) has, for fixed n and $\alpha \geq 1$, the asymptotic behavior

$$[n, n+m]_Q \sim Q + \frac{K'}{2\alpha} \frac{(2\alpha)! n!}{(n+2\alpha)! M^{2\alpha}} \quad (4.18)$$

with $K' = 2\pi c^2 k^{2\alpha-2} I_\alpha^2$. The proof follows from Corollary 4.1, by recognizing that Q_m and $f_m(0)$ have analogous asymptotic behavior [cf. Eq. (3.21)].

5. CONCLUSIONS

It was the aim of this work to study an approximation method able to deal with slow convergent partial wave expansions. With this purpose, the PPA have been proposed. We have applied them to the sequences of finite sums S_m of the partial wave expansions of the scattering amplitude and total cross section, for central potentials with a long range tail. We were able to show that the sequence of $[n, n+m]$ PPA, with fixed n , while converging to the correct values, have a higher rate of convergence than that of the original S_m . The former, represent the rows of the Padé table

$$\begin{array}{ccccccc} [0, 0] & [0, 1] & [0, 2] & [0, 3] & \dots & & \\ [1, 0] & [1, 1] & [1, 2] & [1, 3] & \dots & & \\ [2, 0] & [2, 1] & [2, 2] & [2, 3] & \dots & & \\ \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & & & \end{array},$$

where in the first row, $[0, m] = S_m$. The theorems proved show that we shall have a gain in the asymptotic rate of convergence, when going to the n th row with $n \geq 1$. This gain does not seem very impressive for the forward amplitude, or total cross section, since it is given by the factor $n!/(n+\alpha-1)!$ ($\alpha \geq 2$), but it will be important for nonzero scattering angles, for which the corresponding factors will be of the order of $(1/m)^n$ ($0 < \theta < \pi$) and $(1/m)^{2n}$ ($\theta = \pi$).

Our restrictions on the α exponent of the long range tail of the potentials, are the necessary ones for the convergence of the original sequence S_m . For this kind of potential, the convergence region in the complex $\cos\theta$ plane is restricted to the real segment $-1 \leq \cos\theta \leq 1$. In this work we have not studied the convergence region of the PPA. At least it is the physical region, but by the usual behavior of Padé approximants, we can expect it to be larger. In fact, it is possible to use the PPA as a method for analytical continuation of the Legendre series. This could be an important procedure for Yukawian-type potentials, to continue the scattering amplitude outside the Lehman ellipse.

A numerical study of the convergence properties described in this article, will be reported in a forthcoming paper.¹⁵ We found that, in general, they are those shown by the theorems.¹⁶ It should be remarked, however, that the numerical evidence indicates that the PPA have very good behavior quite before the $S_m(\theta)$ reach their asymptotic form, emphasizing this fact, the importance of the former from the practical point of view. Furthermore, we found fast convergence of the PPA, in the cases of the Coulomb and inverse square potentials, for $\theta \neq 0$, and $\theta = \pi$, respectively, which are not included in our treatment. This suggests that some of the hypotheses imposed in this paper could be released.

Finally, let us note that we have dealt with a particular family of sequences of PPA, i. e., the $[n, n+m]$ with fixed n . However, it is most possible that also other sequences could be well behaved, particularly, as our asymptotic estimates suggest, the $[n, n+m]$

restricted to sufficiently large fixed m , and increasing n .

APPENDIX A: CALCULATION OF $S_{m+r}^{r+1, \alpha}(\theta)$ ($r \geq 0$)

Recalling the recurrence relation for Legendre polynomials¹⁴

$$\frac{(l+1)P_{l+1} + lP_{l-1}}{(l+\frac{1}{2})} = 2 \cos \theta P_l$$

and the definition of $S_m^{0, \alpha}$ [cf. Eq. (3.8)],,

$$S_m^{0, \alpha} = \sum_{l=m+1}^{\infty} \frac{P_l}{(l+\frac{1}{2})^\alpha}$$

one has

$$2 \cos \theta S_m^{0, \alpha} = \sum_{l=m+1}^{\infty} \frac{(l+1)P_{l+1} + lP_{l-1}}{(l+\frac{1}{2})^{\alpha+1}} = \sum_{l=m+1}^{\infty} \frac{P_{l+1} + P_{l-1}}{(l+\frac{1}{2})^\alpha} + \frac{1}{2} \sum_{l=m+1}^{\infty} \frac{P_{l+1} - P_{l-1}}{(l+\frac{1}{2})^{\alpha+1}}. \quad (A1)$$

Furthermore,

$$\begin{aligned} \sum_{l=m+1}^{\infty} \frac{P_{l+1}}{(l+\frac{1}{2})^\alpha} &= \sum_{l=m+2}^{\infty} \frac{P_l}{(l+\frac{1}{2}-1)^\alpha} \\ &= \sum_{l=m+2}^{\infty} \frac{P_l}{(l+\frac{1}{2})^\alpha} \sum_{n=0}^{\infty} \frac{(\alpha+n-1)!}{n!(\alpha-1)!} \frac{1}{(l+\frac{1}{2})^n} \\ &= \sum_{n=0}^{\infty} \frac{(\alpha+n-1)!}{n!(\alpha-1)!} S_{m+1}^{0, \alpha+n} \end{aligned} \quad (A2)$$

and, in an analogous manner, we can see that

$$\sum_{l=m+1}^{\infty} \frac{P_{l-1}}{(l+\frac{1}{2})^\alpha} = \sum_{n=0}^{\infty} \frac{(-1)^n (\alpha+n-1)!}{n!(\alpha-1)!} S_{m-1}^{0, \alpha+n}. \quad (A3)$$

By using (1.2) and (1.3) in Eq. (1.1), we show that

$$S_{m+1}^{0, \alpha} + S_{m-1}^{0, \alpha} = 2 \cos \theta S_m^{0, \alpha} + S_m^{1, \alpha}$$

with

$$S_m^{1, \alpha} = -(\alpha + \frac{1}{2}) \sum_{n=1}^{\infty} \frac{(\alpha+n-1)!}{n! \alpha!} \times [S_{m+1}^{0, \alpha+n} + (-1)^n S_{m-1}^{0, \alpha+n}],$$

and by induction, we show that the $S_m^{i+1, \alpha}$ defined by Eq. (3.15),

$$S_m^{i+1, \alpha} = S_{m+1}^{i, \alpha} + S_{m-1}^{i, \alpha} - 2 \cos \theta S_m^{i, \alpha},$$

is given by the following expression,

$$S_m^{i+1, \alpha} = -(\alpha + \frac{1}{2}) \sum_{n=1}^{\infty} \frac{(\alpha+n-1)!}{n! \alpha!} \times [S_{m+1}^{i, \alpha+n} + (-1)^n S_{m-1}^{i, \alpha+n}].$$

APPENDIX B: HANKEL DETERMINANTS

1. Evaluation of $D_{n+1}^m \{S_{m+k}^{i, \alpha}\}$ in Eq. (4.2)

We note that $D_{n+1}^m \{S_{m+k}^{i, \alpha}\}$ is a determinant of order $n+1$.

Let us consider the case with odd n . In this case the number of columns is even, and we may consider them as arranged in $(n+1)/2$ successive pairs, and operate on a generic one in the following way:

$$\begin{aligned} & \begin{vmatrix} \cdot & S_{m+k}^{i, \alpha} & S_{m+k+1}^{i, \alpha} & \cdot \\ \cdot & S_{m+k+1}^{i, \alpha} & S_{m+k+2}^{i, \alpha} & \cdot \\ \cdot & S_{m+k+1}^{i+1, \alpha} & S_{m+k+2}^{i+1, \alpha} & \cdot \\ \cdot & S_{m+k+2}^{i+1, \alpha} & S_{m+k+3}^{i+1, \alpha} & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \\ & \sim \cos k \theta \sin(k+1)\theta \begin{vmatrix} \cdot & h_k S_m^k & h_k C_m^k & \cdot \\ \cdot & h_k S_{m+1}^k & h_k C_{m+1}^k & \cdot \\ \cdot & h_{k+1} S_{m+1}^{k+1} & h_{k+1} C_{m+1}^{k+1} & \cdot \\ \cdot & h_{k+1} S_{m+2}^{k+1} & h_{k+1} C_{m+2}^{k+1} & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \\ & + \sin k \theta \cos(k+1)\theta \begin{vmatrix} \cdot & h_k C_m^k & h_k S_m^k & \cdot \\ \cdot & h_k C_{m+1}^k & h_k S_{m+1}^k & \cdot \\ \cdot & h_{k+1} C_{m+1}^{k+1} & h_{k+1} S_{m+1}^{k+1} & \cdot \\ \cdot & h_{k+1} C_{m+2}^{k+1} & h_{k+1} S_{m+2}^{k+1} & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \\ & = \sin \theta \begin{vmatrix} \cdot & h_k S_m^k & h_k C_m^k & \cdot \\ \cdot & h_k S_{m+1}^k & h_k C_{m+1}^k & \cdot \\ \cdot & h_{k+1} S_{m+1}^{k+1} & h_{k+1} C_{m+1}^{k+1} & \cdot \\ \cdot & h_{k+1} S_{m+2}^{k+1} & h_{k+1} C_{m+2}^{k+1} & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{vmatrix} \\ & \times \begin{vmatrix} h_0 S_m^0 & h_0 C_m^0 & h_1 S_m^1 & h_1 C_m^1 & \dots \\ h_0 S_{m+1}^0 & h_0 C_{m+1}^0 & h_1 S_{m+1}^1 & h_1 C_{m+1}^1 & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \\ h_j S_{m+j}^j & h_j C_{m+j}^j & h_{j+1} S_{m+j}^{j+1} & h_{j+1} C_{m+j}^{j+1} & \dots \\ h_j S_{m+j+1}^j & h_j C_{m+j+1}^j & h_{j+1} S_{m+j+1}^{j+1} & h_{j+1} C_{m+j+1}^{j+1} & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \end{vmatrix} \end{aligned}$$

with $S_m^n = \sin(\Lambda_m - n\pi/2)$ and $C_m^n = \cos(\Lambda_m - n\pi/2)$. Repeating the procedure for all pairs of columns, the determinant can be reduced to

$$D_{n+1}^m \{S_{m+k}^{i, \alpha}\} \sim (\sin \theta)^{(n+1)/2}$$

and performing a similar artifice with the pairs of rows we get

$$(\sin\theta)^{n+1} \begin{vmatrix} h_0 S_m^0 & h_0 C_m^0 & h_1 S_m^1 & h_1 C_m^1 & \dots \\ h_0 C_m^0 & -h_0 S_m^0 & h_1 C_m^1 & -h_1 S_m^1 & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ h_j S_m^j & h_j C_m^j & h_{j+1} S_m^{j+1} & h_{j+1} C_m^{j+1} & \dots \\ h_j C_m^j & -h_j S_m^j & h_{j+1} C_m^{j+1} & -h_{j+1} S_m^{j+1} & \dots \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{vmatrix}$$

Using now the simple relation between the $\{S_m^n, C_m^n\}$ and the $\{S_m^0, C_m^0\}$, we can rearrange the rows and columns with proper changes of sign, to obtain

$$(-1)^{N+1} (\sin\theta)^{2(N+1)} \begin{vmatrix} h_0 S_m^0 & h_0 C_m^0 & h_1 S_m^0 & h_1 C_m^0 & \dots & h_N C_m^0 \\ h_0 C_m^0 & -h_0 S_m^0 & h_1 C_m^0 & -h_1 S_m^0 & \dots & -h_N S_m^0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ h_N C_m^0 & -h_N S_m^0 & h_{N+1} C_m^0 & -h_{N+1} S_m^0 & \dots & -h_{2N} S_m^0 \end{vmatrix}$$

with $N = (n-1)/2$.

We now subtract from the even columns multiplied by C_m^0 , the next to the right, multiplied by S_m^0 , and proceed in a similar manner with the rows to get, finally,

$$D_{n+1}^m \{S_{m+k}^{i,\alpha}\} \sim (-1)^{N+1} (\sin\theta)^{2(N+1)} \begin{vmatrix} h_0 & 0 & h_1 & 0 & \dots & 0 \\ 0 & -h_0 & 0 & -h_1 & \dots & h_N \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & -h_N & 0 & -h_{N+1} & \dots & -h_{2N} \end{vmatrix}$$

$$= (-1)^{N+1} (\sin\theta)^{2(N+1)} [H_{N+1}^{(0)} \{h_r\}]^2 \quad (B1)$$

For n even, the calculation is somewhat more involved, but following the same approach, we get ($N = n/2$)

$$D_{n+1}^m \{S_{m+k}^{i,\alpha}\} \sim (\sin\theta)^{2N} H_N^{(0)} \{h_r\} H_{N+1}^{(0)} \{h_r\} \sin \Lambda_{m+n}. \quad (B2)$$

By defining $N = n/2$ for even n , and $N = (n-1)/2$ for odd n , we can write Eqs. (B1) and (B2) in the closed expression (4.4).

2. Calculation of $H_{n+1}^{(m)} \{r!\}$ and $H_j^{(0)} \{h_r\}$

By factorizing $(m+h-1)!$ from the h column, for $h = 1, 2, \dots, n+1$, one can see that

$$H_{n+1}^{(m)} \{r!\} = m! (m+1)! \dots (m+n)! \times \begin{vmatrix} 1 & 1 & \dots & 1 \\ (m+1) & (m+2) & \dots & (m+n+1) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \frac{(m+n)!}{m!} & \frac{(m+n+1)!}{(m+1)!} & \dots & \frac{(m+2n)!}{(m+n)!} \end{vmatrix}$$

We now multiply the h row by $(h-1)$ and subtract it from the $h+1$, for $h = n, n-1, n-2, \dots, 3, 2$. Repeating then the procedure, multiplying the h row by $h-2$ and subtracting from the $h+1$ one, for $h = n, n-1, \dots, 4, 3$, and so forth, we obtain

$$H_{n+1}^{(m)} \{r!\} = m! (m+1)! \dots (m+n)! \times \begin{vmatrix} 1 & 1 & \dots & 1 \\ (m+1) & (m+2) & \dots & (m+n+1) \\ (m+1)^2 & (m+2)^2 & \dots & (m+n+1)^2 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ (m+1)^n & (m+2)^n & \dots & (m+n+1)^n \end{vmatrix} = \prod_{p=0}^n (m+p)! p!,$$

where the last equality follows from the fact that the determinant in the first, is a Vandermonde determinant.

We can operate in an analogous manner to show that

$$H_{n+1}^{(0)} \{(m+2r)!!\} = \begin{vmatrix} 1 & 1 & \dots & 1 \\ (m+2) & (m+4) & \dots & (m+2n+2) \\ (m+2)^2 & (m+4)^2 & \dots & (m+2n+2)^2 \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ (m+2)^n & (m+4)^n & \dots & (m+2n+2)^n \end{vmatrix} = 2^{[n(n+1)]/2} \prod_{p=0}^n (m+2p)!! p! \quad (B3)$$

With the result (B3), we can readily calculate $H_j^{(0)} \{h_r\}$. We have [cf. Eq. (4.3)]

$$H_j^{(0)} \{h_r\} = H_j^{(0)} \left\{ \frac{A(\theta)(2\alpha+2j-1)!! (\sin\theta)^j}{(2\alpha-1)!! M^{\alpha+j+1/2}} \right\} = \left(\frac{A(\theta)}{(2\alpha-1)!!} \right)^j \frac{(\sin\theta)^j (j-1)!}{M^{j(\alpha+1/2)}} \times H_j^{(0)} \{2\alpha+2j-1\}!!$$

from which we get Eq. (4.5).

3. Asymptotic evaluation of $H_{n+1}^{(0)} \{\Delta^r S_m(0)\}$ [Eq. (4.10a)]

Using (4.9) one has, by factorization of the determinant,

$$H_{n+1}^{(0)} \{\Delta^r S_m(0)\} \sim H_{n+1}^{(0)} \left\{ \frac{(-1)^r (\alpha+r-2)!}{(\alpha-1)! M^{\alpha+r-1}} \right\} = \frac{H_{n+1}^{(0)} \{\alpha+r-2\}!}{[(\alpha-1)!]^{n+1} M^{(n+\alpha-1) \cdot (n+1)}} = \frac{H_{n+1}^{(\alpha-2)} \{r!\}}{[(\alpha-1)!]^{n+1} M^{(n+\alpha-1) \cdot (n+1)}},$$

where the last equality follows from the property

$$H_n^{(m)} \{S_r\} = H_n^{(0)} \{S_{r+m}\}.$$

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Pseudoscalar transition between a spin- J and a spin- $5/2$ baryon

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The decay width for a spin- J baryon decays into a spin- $5/2$ baryon, and a pseudoscalar meson is expressed in terms of different types of decay amplitudes. The overall ratio among decay amplitudes and the approximate decay width formula are derived by ignoring the higher partial waves.

1. INTRODUCTION

Lee and Chen¹ have pointed out that the SU(3) symmetry is severely broken for the pseudoscalar transition of a spin- $\frac{7}{2}$ baryon into a spin- $\frac{5}{2}$ baryon. Therefore, it is interesting to see whether the SU(3) symmetry is also severely broken for transitions between even higher spin resonances. This is the motivation of the present work in which formulas for the pseudoscalar transition of a spin- J baryon into a spin- $\frac{5}{2}$ baryon are derived for use in testing SU(3) symmetry as long as the experimental data become available.

Owing to parity conservation, the decays in which a spin- J baryon decays into a spin- $\frac{5}{2}$ baryon and a pseudoscalar meson involves three partial waves. Therefore, there are three independent decay amplitudes in the above decay process. The commonly used decay amplitudes are of three types: the Lorentz-invariant coupling constants, the helicity amplitudes, and the partial-wave amplitudes. The Carruthers'² decomposition of the high-spin spinor is used to calculate the decay matrix element with definite helicities, and thus enable us to relate the coupling constants with the helicity amplitudes. The method outlined in Ref. 3 enables us to calculate the partial-wave decay matrix element, and thus enables us to relate the partial-wave amplitudes with the coupling constants. In this way, any type of decay amplitudes can be expressed in terms of other types of decay amplitudes through the above correlations among different types of decay amplitudes. The exact decay width formula can be expressed in terms of coupling constants, or helicity amplitudes or partial-wave amplitudes as we wish.

Since the higher partial wave has the higher centrifugal barrier which lessens the decay probability, it is reasonable to ignore all the higher partial-wave contributions to the decay. In this approximation, simple overall ratios among decay amplitudes, and the approximate decay width formula can be easily derived.

In the present work, the exact decay width formula for a spin- J baryon decays into a spin- $\frac{5}{2}$ baryon and a pseudoscalar meson is given in Sec. 2. The partial-wave expressions are given in Sec. 3. The overall ratios among decay amplitudes and the approximate decay width formula are given in Sec. 4. In the last section we conclude our work.

2. THE DECAY WIDTHS

The three independent Lorentz invariant coupling

constants involved in the decay of a spin- J baryon into a spin- $\frac{5}{2}$ baryon and a pseudoscalar meson are defined by the following expression,

$$\begin{aligned} & \left(\frac{p_0 q_0}{Mm}\right)^{1/2} \langle \frac{5}{2}(q, \lambda') | j_r(0) | J(p, \lambda) \rangle \\ &= \bar{U}_{\mu_1 \mu_2}(q, \lambda') \Gamma' i \gamma_5 \left[\delta_{\mu_1 \nu_1} \delta_{\mu_2 \nu_2} F \right. \\ & \quad \left. + \delta_{\mu_1 \nu_1} \frac{p_{\mu_2} q_{\nu_2}}{m^2} G + \frac{p_{\mu_1} p_{\mu_2} q_{\nu_1} q_{\nu_2}}{m^4} H \right] \\ & \quad \times q_{\nu_3} \cdots q_{\nu_n} \Gamma U_{\nu_1 \cdots \nu_n}(p, \lambda), \end{aligned} \quad (1)$$

where M and m are the masses of the spin- J and the spin- $\frac{5}{2}$ baryons, respectively, λ 's are helicities, $U_{\nu_1 \cdots \nu_n}$ is the spin- J spinor with $n = J - \frac{1}{2}$, and Γ 's are equal to 1 or $i\gamma_5$, depending on the normality of the baryons to be positive or negative, respectively. The normality of a spin- J baryon is defined to be $P(-)^n$ with P as the intrinsic parity. The coupling constants defined in expression (1) can be shown to be real owing to time reversal invariance.

The spin- J spinor can be decomposed² as follows,

$$U_{\nu_1 \cdots \nu_n}(p, \lambda) = \sum_{\lambda', \lambda''} C(1J - 1J; \lambda' \lambda'' \lambda) \mathcal{E}_{\nu_1}(p, \lambda') U_{\nu_2 \cdots \nu_n}(p, \lambda''), \quad (2)$$

where $\mathcal{E}_{\nu}(p, \lambda')$ is the polarization vector. By successive use of the above decomposition, expression (1) can be calculated to be

$$\begin{aligned} & \left(\frac{p_0 q_0}{Mm}\right)^{1/2} \langle \frac{5}{2}(q, \lambda') | j_n(0) | J(p, \lambda) \rangle \\ &= (iN)^{1-\delta} \epsilon^{-1} \left(\frac{(J - \frac{3}{2})! (J + \frac{1}{2})}{(2J - 4)! 2J(J - 1)} \right)^{1/2} \\ & \quad \times q^{J-5/2} \left(\frac{q_0 - \epsilon m}{2m} \right)^{1/2} d_{\lambda \lambda'}^J(\theta) F_{\lambda'}, \end{aligned}$$

with

$$\begin{aligned} F_{5/2} &= \frac{1}{2} \left(\frac{(J + \frac{3}{2})(J + \frac{5}{2})}{2J - 3} \right)^{1/2} F, \\ F_{3/2} &= \left(\frac{J + \frac{3}{2}}{10} \right)^{1/2} \left[\left(\frac{2q_0}{m} - \frac{\epsilon}{2} \right) F - \frac{q^2 M}{m^3} G \right], \\ F_{1/2} &= \left(\frac{J - \frac{1}{2}}{5} \right)^{1/2} \left[\left(\frac{1}{2} + \frac{q_0^2}{m^2} - \frac{\epsilon q_0}{m} \right) F \right. \\ & \quad \left. - \left(\frac{q_0^2 M}{m^4} - \frac{q^2 M}{2m^3} \epsilon \right) G + \frac{q^4 M^2}{m^6} H \right], \end{aligned} \quad (3)$$

$$\frac{F_{\lambda}}{F_{-\lambda}} = -\epsilon.$$

In the above expression, q is the magnitude of the three momentum of the spin- $\frac{5}{2}$ baryon in the overall center of mass system, ϵ is the product of the normalities of the spin- J and the spin- $\frac{5}{2}$ baryons, N is the normality of the spin- J baryon and F_λ is the helicity amplitude. In the derivation of expression (3), the plane formed by the spin quantization axis of the spin- J baryon and \mathbf{q} is chosen as the XZ plane. The corresponding decay width formula can then be easily derived. The expression is

$$\begin{aligned} & \Gamma(J \rightarrow \frac{5}{2} + \pi) \\ &= \frac{1}{2\pi M} \frac{(J - \frac{5}{2})!}{(2J)!} (q_0 - \epsilon m) q^{2J-4} \left\{ \frac{(J + \frac{3}{2})(J + \frac{5}{2})}{8} |F|^2 \right. \\ &+ \frac{(J + \frac{3}{2})(J - \frac{3}{2})}{10} \left| \left(\frac{2q_0}{m} - \frac{\epsilon}{2} \right) F - \frac{q^2 M}{m^3} G \right|^2 \\ &+ \frac{(J - \frac{1}{2})(J - \frac{3}{2})}{5} \left| \left(\frac{1}{2} + \frac{q_0^2}{m^2} - \frac{\epsilon q_0}{m} \right) F \right. \\ &\left. - \left(\frac{q_0}{m} - \frac{\epsilon}{2} \right) \frac{q^2 M}{m^3} G + \frac{q^4 M^2}{m^6} H \right|^2 \left. \right\}. \end{aligned} \quad (4)$$

We note that the above expressions are exact without involving any kinematical and dynamical assumptions except Lorentz invariance.

3. THE PARTIAL-WAVE EXPRESSIONS

The Lorentz invariant decay matrix can be rewritten as

$$\begin{aligned} & \left(\frac{p_0 q_0}{Mm} \right)^{1/2} \langle \frac{5}{2}(q, \lambda') | j_\pi(0) | J(p, \lambda) \rangle \\ &= \langle q, \theta, \phi = 0; \lambda', \lambda_2 = 0 | J(p, \lambda) \rangle', \end{aligned} \quad (5)$$

where $\lambda_2 = 0$ because the pion is spinless, θ is the angle between the spin quantization axis of the decaying baryon and \mathbf{q} , $\phi = 0$ is due to the choice of the XZ plane as mentioned before, the state vector $|J(p, \lambda)\rangle'$ is proportional to $|J(p, \lambda)\rangle$, and the state sector $|q, \theta, \phi = 0; \lambda', \lambda_2 = 0\rangle$ satisfies the orthonormal condition

$$\begin{aligned} & \langle q, \theta', \phi = 0; \lambda', \lambda_2 = 0 | q, \theta, \phi = 0; \lambda'', \lambda_2 = 0 \rangle \\ &= \delta_{\lambda' \lambda''} \delta(\cos \theta' - \cos \theta). \end{aligned} \quad (6)$$

The partial-wave decay matrix element can then be expressed in terms of the Lorentz invariant decay matrix element as follows,

$$\begin{aligned} & \langle LSJ\lambda | J(p, \lambda) \rangle' \\ &= [\pi(2L + 1)]^{1/2} \sum_{\lambda'} C(LSJ; 0\lambda'\lambda') \\ &\times \int d\cos\theta \left[\left(\frac{p_0 q_0}{Mm} \right)^{1/2} \langle \frac{5}{2}(q, \lambda') | j_\pi(0) | J(p, \lambda) \rangle \right] d_{\lambda\lambda'}^J(\theta), \end{aligned} \quad (7)$$

by inserting the complete set of states $|q, \theta, \phi = 0; \lambda', \lambda_2 = 0\rangle$ and using the following expression for the transformation matrix element

$$\begin{aligned} & \langle LSJ\lambda | q, \theta, \phi = 0; \lambda', \lambda_2 = 0 \rangle \\ &= \left(\frac{2L + 1}{4\pi} \right)^{1/2} C(LSJ; 0\lambda'\lambda') d_{\lambda\lambda'}^J(\theta), \end{aligned} \quad (8)$$

which can be derived from the expressions for $\langle LSJ\lambda | JM; \lambda_1 \lambda_2 \rangle$ and $\langle JM; \lambda_1 \lambda_2 | \mathbf{q}; \lambda', \lambda'' \rangle$ given in Ref. (4). Substitute expression (3) for the Lorentz invariant decay matrix element into expression (7), we obtain the lowest partial-wave decay matrix element as follows:

$$\begin{aligned} & \langle LS = \frac{5}{2} J\lambda | J(p, \lambda) \rangle' \\ &= - \frac{(iN)^{(1+\epsilon)/2}}{J} \left[\frac{(J - \frac{3}{2})!(J - \frac{3}{2})\pi}{(2J - 2)!! 2(2\epsilon + 3)(J + \epsilon)} \right]^{1/2} \\ &\frac{q^L F'}{\sqrt{2m} (q_0 + m)^{\epsilon/2}}, \\ &F' = \left((J - \frac{1}{2}) \frac{q_0^2}{m^2} + 2(J + \frac{3}{2} + \epsilon) \frac{q_0}{m} \right. \\ &+ \frac{4J^2 + 8(1 + \epsilon)J + 3(5 + 4\epsilon)}{4(J - \frac{3}{2})} \left. \right) F \\ &- \left((J - \frac{1}{2}) \frac{q_0}{m} + J + \frac{3}{2} + \epsilon \right) \frac{q^2 M}{m^3} G + (J - \frac{1}{2}) \frac{q^4 M^2}{m^6} H, \end{aligned} \quad (9)$$

where $L = J - \frac{5}{2}$ or $J - \frac{3}{2}$, according to whether the baryon's normality changes or not. For the next higher orbital angular momentum, we obtain

$$\begin{aligned} & \langle LS = \frac{5}{2} J\lambda | J(p, \lambda) \rangle' = \left(\frac{(J - \frac{3}{2})!(J + \frac{3}{2})\pi}{(2J - 4)!! 10(J - \epsilon)(J + \epsilon + 1)} \right)^{1/2} \\ &\times \frac{(iN)^{(1+\epsilon)/2}}{2J + \epsilon - 1} \frac{q^L}{\sqrt{2m} (q_0 + m)^{\epsilon/2}} \frac{G'}{m^2}, \\ &G' = \left((2J - 1) \frac{q_0}{m} + (2J + 2\epsilon + 7) \right) \frac{m}{q_0 + m} F \\ &- \left((2J - 1) \frac{q_0}{m} + 4 + \epsilon \right) \frac{M}{m} G + (2J - 1) \frac{q^2 M^2}{m^4} H, \end{aligned} \quad (10)$$

where $L = J - \frac{1}{2}$ or $J + \frac{1}{2}$, depending upon whether the baryon's normality changes or not. For the highest orbital angular momentum, we obtain

$$\begin{aligned} & \langle LS = \frac{5}{2} J\lambda | J(p, \lambda) \rangle' \\ &= - \left[\frac{(J - \frac{3}{2})!(J - \frac{1}{2})(J + \frac{3}{2})(J + \frac{5}{2})\pi}{(2J)!! (3 - 2\epsilon)(J + 1)(J + \epsilon + 1)} \right]^{1/2} \\ &\times \frac{(iN)^{(1+\epsilon)/2}}{\sqrt{2m} (q_0 + m)^{\epsilon/2}} \frac{H'}{m^4}, \end{aligned} \quad (11)$$

$$H' = \frac{m^2}{(q_0 + m)^2} F - \frac{M}{q_0 + m} G + \frac{M^2}{m^2} H,$$

where $L = J + \frac{3}{2}$ or $J + \frac{5}{2}$, according to whether the baryon's normality changes or not. In the above expressions, F' , G' , and H' are the lowest, next higher, and the highest partial-wave amplitudes, respectively.

The decay width when expressed in terms of partial-wave decay matrix elements takes the following form,

$$\Gamma(J \rightarrow \frac{5}{2} + \pi) = \frac{mq}{8\pi^2 M} \sum_L |\langle LS = \frac{5}{2} J\lambda | J(p, \lambda) \rangle'|^2. \quad (12)$$

Substituting expressions (9), (10), and (11) into expression (12), we can express the decay width in terms of the partial-wave amplitudes as follows,

$$\begin{aligned} & \Gamma(J \rightarrow \frac{5}{2} + \pi) \\ &= \frac{(J - \frac{3}{2})!}{(2J - 4)!! J(J - 1)} \frac{(q_0 - \epsilon m) q^{2J-4}}{64\pi M} \left\{ \frac{J - \frac{3}{2}}{(3 + 2\epsilon)J(J + \epsilon)} \right. \\ &\times |F'|^2 + \frac{2J + 3}{5(2J + \epsilon - 1)(2J + \epsilon + 3)} \frac{q^4}{m^4} |G'|^2 \\ &+ \frac{(J - \frac{1}{2})(J + \frac{3}{2})(J + \frac{5}{2})}{(3 - 2\epsilon)(J + 1)(J + \epsilon + 1)} \frac{q^8}{m^8} |H'|^2 \left. \right\}. \end{aligned} \quad (13)$$

It can be easily checked that expression (13) is identical to expression (4).

4. APPROXIMATION

Since the higher partial wave involves the higher centrifugal barrier which lessens the decay probability, it is reasonable to ignore the higher partial wave contributions. Mathematically, the complete neglect of the higher partial-wave contributions corresponds to setting the higher partial wave amplitudes equal to zero, i. e., $G' = H' = 0$. Under this approximation, all decay amplitudes become proportional to one another. The overall ratio among them is calculated from the expressions (9), (10), (11), and (3). The result is

$$\begin{aligned}
 F : G : H : F_{5/2} : F_{3/2} F_{1/2} : F' \\
 = 1 : \frac{2m^2}{(q_0 + m)M} : \frac{m^4}{(q_0 + m)^2 M^2} : \left(\frac{(J + \frac{3}{2})(J + \frac{5}{2})}{J - \frac{3}{2}} \right)^{1/2} \\
 : \frac{1}{2\sqrt{10}} (4 - \epsilon)(J + \frac{3}{2})^{1/2} \\
 : \frac{1}{2\sqrt{5}} (3 - 2\epsilon)(J - \frac{1}{2})^{1/2} : \frac{4J(J + \epsilon)}{J - \frac{3}{2}}. \quad (14)
 \end{aligned}$$

From the above ratio (14), all decay amplitudes can be calculated, if one of them is known. The corresponding expression for the decay width takes a very simple form,

$$\begin{aligned}
 \Gamma(J \rightarrow \frac{5}{2} + \pi) = \frac{(J - \frac{5}{2})! [(1 + \epsilon)J + 2]}{(2J - 4)! [(1 + \epsilon)J - 2\epsilon]} \\
 \times \frac{(q_0 - \epsilon m) q^{2J-4}}{(12 + 8\epsilon)\pi M} |F|^2, \quad (15)
 \end{aligned}$$

which are derived from the expressions (13) and (14).

5. CONCLUSIONS AND DISCUSSION

In the present paper, we derive the exact expression for the decay width of a spin- J baryon decaying into a spin- $\frac{5}{2}$ baryon and a pseudoscalar meson. The exact correlations between coupling constants, helicity amplitudes, and partial-wave amplitudes are also given. We also derive the overall ratio among decay amplitudes and a simple decay width formula under the approximation which ignores the higher partial waves.

We note that all decay amplitudes defined in this paper are real, owing to time reversal invariance. In order to test SU(3) symmetry the Lorentz-SU(3) invariant coupling constants are obtained by dividing the coupling constants defined in expression (1) by the proper SU(3) Clebsch-Gordan coefficient. Then expression (15) enables us to predict all decays between the interested multiplets as long as one decay width is known.

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Electromagnetic radiation near black holes and neutron stars

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Analytic solutions to Maxwell's equations in the Schwarzschild geometry are given. These are obtained by differentiating a single superpotential, which is valid (and bounded) at and everywhere outside the gravitational radius. The results have application to black-hole and neutron-star electrodynamics.

I. INTRODUCTION

Several techniques have been used by a number of authors including Wheeler,¹ Mashhoon,² Mo and Papas,³ Stephani,⁴ and Cohen and Kegeles⁵ to reduce the electromagnetic field equations in Schwarzschild space to a single radial wave equation. Its solutions yield arbitrary dynamic multipoles with general azimuthal dependence,²⁻⁵ and furthermore may be considered as the radial factor in a Debye potential, in terms of which the physical **E** and **B** components may be constructed explicitly by differentiation.³⁻⁵ In spite of the advantage of analytic solutions for the radial equation, especially in the Debye potential picture where derivatives of the function appear in the physical field, no known special functions solve the equation except in the static limit.⁵⁻⁷ Thus, previous work has treated the equation by approximation methods²⁻³ or numerically.^{2,8,9} It is the purpose of this paper to give analytic solutions to the radial wave equation.

In addition to the radial equation derived in Refs. 1-5, an equivalent equation corresponding to a spherical decomposition of the field has been obtained by Bardeen and Press,¹⁰ Teukolsky,¹¹ and Cohen and Kegeles.⁵ In Ref. 5, the viewpoint is again that the solutions are interpreted as Debye potentials which yield the field components by differentiation. However, it is the spherical radial equation of Refs. 1-5 which is treated in the present work.

This equation is

$$A^2 \partial_r (A^2 \partial_r R) + [k^2 - l(l+1)r^{-2}A^2]R = 0, \quad (1)$$

where $A^2 = 1 - 2Mr^{-1}$, ∂_r denotes differentiation with respect to r , and M is the mass. In the orthonormal frame

$$\omega^0 = Adt, \quad \omega^1 = Bdr, \quad \omega^2 = rd\theta, \quad \omega^3 = r \sin\theta d\phi, \quad (2)$$

where $B^{-2} = A^2$, the physical electromagnetic field components are⁵

$$B_1 = l(l+1)r^{-2} \exp(-ikt) R_{l,k}(r) Y_l^m(\theta, \phi),$$

$$B_2 = Ar^{-1} \exp(-ikt) \partial_r R_{l,k} \partial_\theta Y_l^m,$$

$$B_3 = i m A r^{-1} \exp(-ikt) \partial_r R_{l,k} Y_l^m / \sin\theta, \quad (3)$$

$$E_1 = 0, \quad E_2 = -km B r^{-1} \exp(-ikt) R_{l,k} Y_l^m / \sin\theta,$$

$$E_3 = -ik B r^{-1} \exp(-ikt) R_{l,k} \partial_\theta Y_l^m.$$

These are the magnetic multipoles; the electric multipoles can be obtained via the duality rotation $E \rightarrow B$, $B \rightarrow -E$.

The remainder of this paper will be devoted to solving Eq. (1) and studying the properties of the solutions $R_{l,k}(r)$.

II. COORDINATE TRANSFORMATIONS

Equation (1) takes a useful form when the radius is expressed as a multiple of the gravitational radius $2M$,

$$\partial_x [(1-x^{-1})\partial_x R] + [\alpha^2(1-x^{-1})^{-1} - \lambda x^{-2}]R = 0, \quad (4)$$

where

$$\alpha = 2Mk, \quad \lambda = l(l+1), \quad \text{and } x = r/2M. \quad (5)$$

When expressed in terms of the variable¹²

$$y = x + \ln(x-1), \quad (6)$$

the equation takes the simple form

$$\partial_y^2 R + (\alpha^2 - \lambda g)R = 0, \quad (7)$$

where $g = (x-1)x^{-3}$ (cf. Ref. 13 for a treatment of the scalar field). The maximum value of g (at $x = \frac{3}{2}$) is $\frac{4}{27}$. When $\alpha^2 > 4\lambda/27$, the solution has a wave character in the entire region $1 < x < \infty$. But if $\alpha^2 < 4\lambda/27$, there are two transition points (for $1 < x$). Between these transition radii the solution takes the form of a sum of decaying and growing exponentials of varying growth rate.² (In the case of gravitational perturbations this barrier effect was noted by Regge and Wheeler¹² and by Vishveshwara.¹⁴) The transition points, which can be found by solving for x in the expression

$$g = (x-1)x^{-3} = \alpha^2/\lambda, \quad (8)$$

are located at $x \approx 1.01$ and 10 for a typical pulsating neutron star^{15,16} of mass $1.2 m_\odot$ and pulsation period 0.5 ms. Since the radius of such a star is ~ 10 km, typical neutron star surfaces are in the region of exponential dependence, which extends out to about 40 km or ~ 4 neutron star radii.

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III. INTEGRAL EQUATION

An integral equation¹⁷ for R can be obtained from Eq. (7), e. g., via Green's function techniques. If the λg term is moved to the right side of Eq. (7), the equation becomes that of a harmonic oscillator with an inhomogeneous driving term which is a function of R ,

$$\partial_y^2 R + \alpha^2 R = \lambda g R. \quad (9)$$

Proceeding as if the inhomogeneous term is known and solving via Green's functions, we obtain the integral equation of the Volterra type,

$$R(y) = f(y) + \lambda \alpha^{-1} \int_{y_0}^y \sin \alpha(y - \eta) g(\eta) R(\eta) d\eta, \quad (10)$$

where $f(y)$ is the homogeneous solution

$$f(y) = C_1 \exp(i\alpha y) + C_2 \exp(-i\alpha y). \quad (11)$$

By using Eq. (6), this integral equation can be expressed in terms of x ,

$$R(x) = f(y(x)) + \lambda \alpha^{-1} \int_{x_0}^x \sin \alpha[y(x) - y(\xi)] R(\xi) \xi^{-2} d\xi \quad (12)$$

($\xi \rightarrow x$) where $0 \leq x_0 \leq \infty$ and $0 \leq x \leq \infty$. Equation (12) can be solved via iteration. The procedure involves the kernel

$$K(x, \xi) = \lambda \alpha^{-1} \xi^{-2} \sin \alpha[y(x) - y(\xi)] \quad (13)$$

as follows: Let the zeroth approximation for R vanish, $R_0(x) = 0$, which with Eq. (13) implies that the $(n+1)$ st approximation is related to the n th via

$$R_{n+1}(x) = R_1(x) + \int_{x_0}^x K(x, \xi) R_n(\xi) d\xi, \quad (14)$$

where $R_1(x) = f(y(x))$.

That the iteration procedure converges can be shown by induction. First we show that the first approximation is bounded by

$$\begin{aligned} |R_1(x)| &= |f(y(x))| = |C_1 \exp(i\alpha y) + C_2 \exp(-i\alpha y)| \\ &\leq |C_1| + |C_2| \equiv D \end{aligned} \quad (15)$$

by the triangle inequality. Next we show that the difference between the $(n+1)$ st and the n th approximations is bounded by

$$|R_{n+1}(x) - R_n(x)| \leq D b^n (n!)^{-1} |x_0^{-1} - x^{-1}|^n, \quad (16)$$

where $b \equiv \lambda |\alpha|^{-1}$. The proof by induction is as follows: From Eq. (15) we see that Eq. (16) is true for $n=0$. If we assume that it is true for n we find

$$\begin{aligned} &|R_{n+2}(x) - R_{n+1}(x)| \\ &= \left| \int_{x_0}^x d\xi K(x, \xi) [R_{n+1}(\xi) - R_n(\xi)] \right|. \end{aligned}$$

Use of Eqs. (13) and (16) brings this into the form

$$\begin{aligned} &\leq \left| \int_{x_0}^x d\xi b \xi^{-2} \sin \alpha[y(x) - y(\xi)] \right. \\ &\quad \times D b^n (n!)^{-1} |x_0^{-1} - \xi^{-1}|^n \\ &\leq \left| \int_{x_0}^x d(\xi^{-1}) |x_0^{-1} - \xi^{-1}|^n D b^{n+1} (n!)^{-1} \right. \\ &\quad \times \sin \alpha[y(x) - y(\xi)] \end{aligned}$$

$$\begin{aligned} &\leq D b^{n+1} [(n+1)!]^{-1} |x_0^{-1} - x^{-1}|^{n+1} \\ &\quad \times |\sin \alpha[y(x) - y(\xi)]|_{\max} \\ &\leq D b^{n+1} [(n+1)!]^{-1} |x_0^{-1} - x^{-1}|^{n+1} \end{aligned}$$

which implies that it is true for all n . This establishes Eq. (16).

It is possible to obtain the upper bound of the $(N+1)$ st approximation using Eq. (16) as follows:

$$R_{N+1}(x) = R_1(x) + \sum_{n=1}^N [R_{n+1}(x) - R_n(x)] \quad (17a)$$

$$\leq D + D \sum_{n=1}^N b^n (n!)^{-1} |x_0^{-1} - x^{-1}|^n. \quad (17b)$$

In the limit $N \rightarrow \infty$ we obtain the bound on R ,

$$R(x) \leq D \exp(b |x_0^{-1} - x^{-1}|), \quad (18)$$

where $b = l(l+1)(2Mk)^{-1}$.

Thus Eq. (18) shows that for $k \neq 0$, the solution is bounded everywhere in the range $1 \leq x \leq \infty$; the solution does not diverge anywhere in this range, not even at $x=1$.

IV. SERIES SOLUTION

In this section we construct a series solution valid in the range $1 \leq x < \infty$. This cannot be done by expanding Eq. (4) around $x=1$ because the series solution converges only in a circle out to the nearest singularity. Since $x=0$ is also a singular point of the equation, such a series solution converges only in the region $1 \leq x \leq 2$ and thus is not useful for our purposes.

This difficulty can be circumvented by mapping the region $1 \leq x < \infty$ into the region from 0 to 1 and by mapping the region $0 < x \leq 1$ into the region 1 to ∞ . Then the series solution in the new space covers the desired interval when mapped back into the original space.

The desired transformation is $z = x^{-1}$. In this variable, the differential equation (4) takes the form

$$-z^2 \partial_z [(z-1)z^2 \partial_z R(z)] + (\alpha^2(1-z)^{-1} - \lambda z^2) R = 0, \quad (19)$$

or the alternate form

$$\partial_z^2 R + p(z) \partial_z R + q(z) R = 0. \quad (20)$$

Here we have

$$p(z) = (3z-2)z^{-1}(z-1)^{-1} = (z-1)^{-1} + 2z^{-1} \quad (21a)$$

and

$$q(z) = \alpha^2 z^{-4} (z-1)^{-2} + \lambda z^{-2} (z-1)^{-1}. \quad (21b)$$

In terms of the parameter $\sigma = 1 - z$, Eqs. (21a) and (21b) become

$$p(\sigma) = -\sigma^{-1} + 2 \sum_{n=0}^{\infty} \sigma^n \equiv \sum_{n=-1}^{\infty} p_n \sigma^n, \quad (22a)$$

$$\begin{aligned} q(\sigma) &= \alpha^2 6^{-1} \sigma^{-2} \sum_{n=0}^{\infty} (n+1)(n+2)(n+3) \sigma^n - \lambda \sigma^{-1} \sum_{n=0}^{\infty} (n+1) \sigma^n \\ &\equiv \sum_{n=-2}^{\infty} q_n \sigma^n. \end{aligned} \quad (22b)$$

A Frobenius series expansion¹⁸

$$R(\sigma) = \sum_{n=0}^{\infty} \nu_n \sigma^{n+\beta} \quad (23)$$

converges in the range $|\sigma| < 1$. Since $\sigma = 1 - z = 1 - x^{-1}$, we have $|1 - x^{-1}| < 1$ and thus the series is valid for $1 \leq x < \infty$.

Substituting Eq. (23) into Eq. (19) gives

$$0 = \sigma^\beta \sum_{n=0}^{\infty} \nu_n [(n+\beta)(n+\beta-1)\sigma^{n-2} - (n+\beta)\sigma^{n-1} \sum_{m=-1}^{\infty} p_m \sigma^m + \sigma^n \sum_{m=-2}^{\infty} q_m \sigma^m]. \quad (24)$$

The vanishing of the $\sigma^{\beta-2}$ term gives $\beta^2 = -\alpha^2$ while the remainder of the ν_n are related by

$$\nu_k (k+\beta)(k+\beta-1) - \sum_{n=0}^k \nu_n (n+\beta) p_{k-1-n} + \sum_{n=0}^k \nu_n q_{k-2-n} = 0. \quad (25)$$

Hence we obtain the recursion relations

$$\nu_k = k^{-1} (k+2\beta)^{-1} \sum_{n=0}^{k-1} [2(n+\beta) - q_{k-n-2}] \nu_n \quad (26a)$$

with

$$q_{n-2} = \alpha^2 \delta^{-1} (n+1)(n+2)(n+3) - n\lambda, \quad (26b)$$

subject to $\beta = \pm i\alpha$. If we set $\nu_0 = 1$, then we find $\nu_1 = (4\beta^2 + 2\beta + \lambda)(2\beta + 1)^{-1}$, etc., with $\nu_n(i\alpha) = \nu_n(-i\alpha)$. In terms of the variable x , the series solutions are

$$R^{(1)}(x) = (1 - x^{-1})^{i\alpha} \sum_{n=0}^{\infty} \nu_n(i\alpha) (1 - x^{-1})^n \quad (27a)$$

and

$$R^{(2)}(x) = (1 - x^{-1})^{-i\alpha} \sum_{n=0}^{\infty} \nu_n(-i\alpha) (1 - x^{-1})^n. \quad (27b)$$

These solutions are valid in the range $1 \leq x < \infty$ and the general solution $R(x)$ is a linear combination of these,

$$R(x) = A_1 R^{(1)}(x) + A_2 R^{(2)}(x). \quad (28)$$

Note that for $\alpha = 2kM \neq 0$, the solution does not diverge in the range $1 \leq x < \infty$ anywhere, not even at $x = 1$. This result is in agreement with that of Eq. (18).

V. FAR FIELD SOLUTION

In this section we give the far field solution to the integral equation (12). This can be done by letting $x_0 \rightarrow \infty$ and gives

$$R^{(*)}(x) = \exp[i\alpha y(x)] + \lambda \alpha^{-1} \int_x^{\infty} \sin \alpha [y(\xi) - y(x)] \times R^{(*)}(\xi) \xi^{-2} d\xi. \quad (29)$$

Here $y(x)$ is given by Eq. (6) and we have taken for f the outgoing wave at infinity $f = \exp[i\alpha y(x)]$. The definition

$$f_n(x) \equiv R_{n+1}(x) - R_n(x) \quad (30)$$

brings Eq. (17a) into the form

$$R(x) = \sum_{n=0}^{\infty} f_n(x) \quad (31)$$

in the limit $N \rightarrow \infty$. From Eqs. (30) and (14) we have

$$f_0(x) = R_1(x) = f(y(x)) = \exp[i\alpha y(x)], \quad (32)$$

and

$$f_{n+1}(x) = - \int_x^{\infty} K(x, \xi) f_n(\xi) d\xi, \quad (33)$$

where $K(x, \xi)$ is given by Eq. (13).

The above method of solution is equivalent to

$$R(x) = R_1(x) + \int_x^{\infty} K^*(x, \xi) R_1(\xi) d\xi, \quad (34a)$$

where

$$K^*(x, \xi) \equiv \sum_{n=1}^{\infty} K_n(x, \xi), \quad (34b)$$

$$K_1(x, \xi) \equiv -K(x, \xi) = b \xi^{-2} \sin \alpha [y(\xi) - y(x)], \quad (34c)$$

and

$$K_{n+1}(x, \xi) \equiv \int_x^{\xi} K_1(x, \eta) K_n(\eta, \xi) d\eta. \quad (34d)$$

A straightforward method of showing this is to convert the Volterra type equation into a Fredholm type and then to iterate successively.¹⁹ In other words, substitute the expression for $R(y)$ in Eq. (10) for $R(\eta)$ and obtain an expression of order λ^2 , and repeat to obtain an expression of order λ^n . The series (31) and (34b) converge uniformly for all $x \geq 1$ [at least as well as $\sum_{n=0}^{\infty} (b/x)^n (n!)^{-1} = \exp(b/x)$ since $D = 1$ in Eq. (18)]. For large x , we obtain the solution to the differential equation (7),

$$R^{(*)}(x) = \exp[i\alpha [x + \ln(x-1)]] [1 + O(x^{-1}) + \dots], \quad (35)$$

since $y(x) = x + \ln(x-1)$. Only $R_2(x)$ needs to be considered for this estimate since higher approximation gives extra terms which fall off faster than x^{-1} .

VI. CONNECTION CONSTANTS

The constants connecting the series solution (28) with the far field solution can be found by using Eq. (29). In exponential form, Eq. (29) becomes

$$R^{(*)}(x) = \exp[i\alpha y(x)] + \lambda(2i\alpha)^{-1} \times \{ \exp[-i\alpha y(x)] \int_x^{\infty} \exp[i\alpha y(\xi)] R^{(*)}(\xi) \xi^{-2} d\xi - \exp[i\alpha y(x)] \int_x^{\infty} \exp[-i\alpha y(\xi)] R^{(*)}(\xi) \xi^{-2} d\xi \}, \quad (36)$$

where $R^{(*)}(\xi)$ is given by Eq. (29) and $y(x) = x + \ln(x-1)$.

Since the \int_x^{∞} can be replaced by $\int_1^{\infty} - \int_1^x$, we can use the inequalities (18) and $|\exp[\pm i\alpha y(\xi)]| \leq 1$ to obtain

$$R(x) = \exp[i\alpha y(x)] [1 + i\lambda(2\alpha)^{-1} \int_1^{\infty} \exp[-i\alpha y(\xi)] R(\xi) \xi^{-2} d\xi + O(x-1)] - \exp[-i\alpha y(x)] [i\lambda(2\alpha)^{-1} \times \int_1^{\infty} \exp[i\alpha y(\xi)] R(\xi) \xi^{-2} d\xi + O(x-1)]. \quad (37)$$

Comparing this with Eq. (28) [and noting that $(1 - x^{-1})^{i\alpha} = \exp[i\alpha \ln(x-1)]$] for $x \approx 1$ gives the connection constants

$$A_1 = \exp(i\alpha) \left[1 + i\lambda(2\alpha)^{-1} \int_1^\infty \exp[-i\alpha y(\xi)] \xi^{-2} \times \sum_{n=0}^\infty f_n(\xi) d\xi \right], \quad (38)$$

$$A_2 = -\exp(-i\alpha) \left[i\lambda(2\alpha)^{-1} \int_1^\infty \exp[i\alpha y(\xi)] \times \sum_{n=0}^\infty f_n(\xi) \xi^{-2} d\xi \right]$$

which provide the relation between the near and far field solutions.

VII. ASYMPTOTIC EXPANSIONS

In this section we use an alternative procedure²⁰ to obtain a few terms in the asymptotic expansion. Carrying out the indicated differentiations in Eq. (4) gives

$$(1 - x^{-1})^2 \partial_x^2 R + (1 - x^{-1}) x^{-2} \partial_x R + [\alpha^2 - \lambda x^{-2} (1 - x^{-1})] R = 0 \quad (39a)$$

or

$$\partial_x^2 R + g_1(x) \partial_x R + g_2(x) R = 0, \quad (39b)$$

with

$$g_1(x) \equiv (x-1)^{-1} - x^{-1}, \quad g_2(x) \equiv \alpha^2 x^2 (x-1)^{-2} - \lambda g_1(x).$$

This equation has singularities at $x=0, 1$, and ∞ .

The procedure to be used here is to factor out certain singular parts of the solution and then to work with the remaining parts. The substitution

$$R(x) = (x-1)^\rho U(x) \quad (40)$$

reduces the order of the singularity at $x=1$ and gives the equation

$$\partial_x^2 U + P_1(x) \partial_x U + P_2(x) U = 0 \quad (41a)$$

with

$$P_1(x) \equiv (1 + 2\rho x) x^{-1} (x-1)^{-1} \\ P_2(x) \equiv -[\rho^2 x(x+1) + \rho + \lambda] x^{-1} (x-1)^{-1}, \quad (41b) \\ \rho = \pm i\alpha.$$

There is an essential singularity at infinity as can be seen from Eqs. (20) and (21). This singularity can be handled by factoring out of the solution the predominant exponential behavior $\exp(\pm\rho x)$, and using the substitution

$$U(x) = \exp(\rho x) \mu(x) \quad (42)$$

in Eq. (41). The resulting equation is

$$\partial_x^2 \mu + \bar{P}_1(x) \partial_x \mu + \bar{P}_2(x) \mu = 0 \quad (43a)$$

with

$$\bar{P}_1 \equiv 2\rho + P_1 = (1 + 2\rho x) x^{-1} (x-1)^{-1}, \\ \bar{P}_2 \equiv \rho^2 + \rho P_1 + P_2 = -\lambda x^{-1} (x-1)^{-1}. \quad (43b)$$

Substitution into Eq. (43) of the Laurent series expansion

$$\mu(x) = 1 + \sum_{n=1}^\infty \mu_n x^{-n} \quad (44)$$

gives

$$\sum_{n=0}^\infty \mu_n [n(n+1)x^{-n-2} - nx^{-n-1} \bar{P}_1 + x^{-n} \bar{P}_2] = 0, \quad (45a)$$

where we use the expansions

$$\bar{P}_1 = (2\rho + x^{-2}) \sum_{n=0}^\infty x^{-n} \equiv \sum_{n=0}^\infty \bar{P}_{1,n} x^{-n}, \quad (45b)$$

$$\bar{P}_2 = -\lambda x^{-2} \sum_{n=0}^\infty x^{-n} \equiv \sum_{n=2}^\infty \bar{P}_{2,n} x^{-n}.$$

Equating the coefficients of equal powers of x^{-n} to zero gives

$$-2\rho\mu_1 - \lambda\mu_0 = 0 \quad (46a)$$

from x^{-2} , and gives for $n > 0$

$$n(n+1)\mu_n - \sum_{k=1}^{n+1} k\mu_k \bar{P}_{1,n-k+1} - \lambda \sum_{k=0}^n \mu_k = 0. \quad (46b)$$

Hence we find:

$$\mu_1 = -\lambda(2\rho)^{-1}, \\ \mu_2 = \lambda(\lambda-2)(8\rho^2)^{-1}, \\ \mu_3 = -\lambda(48\rho^3)^{-1}[(\lambda-2)(\lambda-6) - 12\rho], \\ \mu_4 = \lambda(384\rho^4)^{-1}[(\lambda-2)(\lambda-6)(\lambda-12) - 60\rho(\lambda-4)], \quad (47)$$

which gives the resulting asymptotic expansion

$$R(x) = (x-1)^\rho \exp(\rho x) \left[1 + \sum_{n=1}^\infty \mu_n x^{-n} \right]. \quad (48)$$

VIII. DISCUSSION

A power series solution to the Schwarzschild electromagnetic radial equation covering the entire region from the gravitational radius to infinity has been derived and is given by Eqs. (27a) and (27b) of Sec. IV. In addition, the asymptotic solution is given in Sec. V and a method for matching this far-field solution to the series expansion is presented in Sec. VI; use of this matching technique avoids the necessity of summing increasingly many terms of the series for asymptotically large radius to obtain a given accuracy. The present method provides an alternative to the conventional direct numerical integration of the differential equation with the advantage that the radial dependence is obtained analytically.

An extension of the Debye potential formalism to other spin values has led to similar scalar wave equations for neutrino and gravitational perturbations of space-times.²¹ The methods of this paper can be used to solve the resulting neutrino and gravitational radial equations (see also Refs. 12, 14, and 22-24) for the Schwarzschild black hole or neutron star in close analogy with the electromagnetic case.

The analytic solutions of this paper are useful for astrophysical calculations involving these types of fields near nonrotating black holes and neutron stars.²⁵

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Semiclassical quantization of a field theoretic model in any number of spatial dimensions

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The semiclassical canonical quantization of the nonrelativistic logarithmic theory is done in any number of spatial dimension d . Instead of the usual expansion of the Hamiltonian about the classical fields, we propose an alternative route to semiclassical quantization by making an expansion around the charge operator. When we take the value $d = 0$ in the energy expression, the exact zero-dimensional spectrum is obtained. The mechanism of confinement characteristic of these logarithmic theories is also discussed.

I. INTRODUCTION

Recently a lot of effort has been concentrated in the study of semiclassical methods of quantization in field theory.¹⁻⁹ By using these nonperturbative instruments the spectra of a large number of $(1 + 1)$ -dimensional models were obtained. Here we succeed in performing the semiclassical quantization of a theory in any number of spatial dimensions.

The model which we quantize is just the nonrelativistic logarithmic theory proposed by Birula and Mycielski.¹⁰

The relativistic logarithmic theory¹⁰⁻¹³ has been intensively studied by us. In Ref. 11 the stability of its soliton-like solutions was discussed, whereas the set of these solutions was considerably enlarged in Ref. 12. In Ref. 13 we pointed out the remarkable fact that the logarithmic theories exhibit confinement. Unfortunately, up to now we have not succeeded in quantizing the relativistic version of the model—the main difficulty coming from the question of renormalizability of theories with logarithmic nonlinearities.

The nonrelativistic logarithmic theory shares the most interesting features of the relativistic one (solitons and confinement), and—at least up to WKB quantization—it does not display any trouble concerning to renormalization. This is the reason for studying it in this paper.

The model is presented in Sec. II. There the stability equation is obtained and solved, leading to a discrete set of stability angles. The mechanism of confinement is discussed in the context of this non relativistic theory.

In Sec. III we compute the static spectrum of the model by using the DHN quantization formula.^{1,2,7} The computation is done in any number of spatial dimensions. We show that, extending our energy formula to dimension zero, the exact zero-dimensional spectrum is obtained.

The canonical quantization of the theory is performed in Sec. IV. There, besides the static spectrum, the kinetic part of the energy is also obtained. Since we use collective variables, our method is similar to

those of Refs. 4–6. But, an important difference deserves to be pointed out: instead of expanding—the Hamiltonian about the *classical field* (soliton), the expansion is done around a *leading operator*. In the present case the suitable leading operator is just the charge. So, our approach is expected to hold only in the computation of the energies of large charge states. The canonical commutation relations are satisfied in a semiclassical sense.

Conclusions are left to Sec. V, while three appendixes complement some calculations of the text.

II. THE MODEL: SOLITONS, STABILITY AND CONFINEMENT

The model that we investigate here is defined by the following Lagrangian density¹⁰:

$$\mathcal{L}(\varphi^\dagger, \varphi) = i\varphi^\dagger \partial_t \varphi - U(\varphi^\dagger, \varphi), \quad (2.1)$$

where φ represents a complex scalar field and $U(\varphi^\dagger, \varphi)$ is given by

$$U(\varphi^\dagger, \varphi) = \frac{1}{2m} \partial_{\mathbf{x}} \varphi^\dagger \partial_{\mathbf{x}} \varphi - \frac{1}{2ml^2} \varphi^\dagger \varphi [\ln(\varphi^\dagger \varphi a^d) - 1]. \quad (2.2)$$

In expression (2.2), l , $1/m$, and a are dimensional parameters while d stands for the number of spatial dimensions.

The Euler–Lagrange equation resulting from (2.1) is

$$i\partial_t \varphi + \frac{1}{2m} \partial_{\mathbf{x}}^2 \varphi + \frac{1}{2ml^2} \ln(\varphi^\dagger \varphi a^d) \varphi = 0. \quad (2.3)$$

The energy associated with a certain field $\varphi(\mathbf{x}, t)$ is given by

$$E = \int d^d \mathbf{x} U(\varphi^\dagger, \varphi), \quad (2.4)$$

whereas the other conserved quantity (the charge) will be

$$Q = \int d^d \mathbf{x} \varphi^\dagger(\mathbf{x}, t) \varphi(\mathbf{x}, t). \quad (2.5)$$

We are interested in the following family of classical solutions (solitons):

$$\varphi_\omega(\mathbf{x}, t) = A(\omega) \exp(-i\omega t - \mathbf{x}^2/2l^2). \quad (2.6)$$

Plugging the field (2.6) into the equation of motion (2.3), we obtain the allowed values of $A(\omega)$:

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$$A(\omega) = a^{-d/2} \exp(d/2 - m l^2 \omega). \quad (2.7)$$

The solution (2.6) describes an spherically symmetric extended object on its proper rest frame. The energy and the charge associated with this classical particle are given respectively by

$$E_d(\omega) = (\sqrt{\pi} l/a)^d (\omega + 1/2 m l^2) \exp(d - 2 m l^2 \omega), \quad (2.8)$$

and

$$Q(\omega) = (\sqrt{\pi} l/a)^d \exp(d - 2 m l^2 \omega). \quad (2.9)$$

A. Stability

In order to study the infinitesimal stability^{7,11} of our particle, we add to the classical solutions (2.6) a small fluctuation

$$\varphi(\mathbf{x}, t) = \varphi_\omega(\mathbf{x}, t) + \exp(-i\omega t) \eta(\mathbf{x}, t). \quad (2.10)$$

Using this representation for $\varphi(\mathbf{x}, t)$ in the equation of motion (2.3) and retaining terms up to first order in $\eta(\mathbf{x}, t)$, we obtain the linearized stability equation:

$$\left[i\partial_t + \frac{1}{2m} \partial_{\mathbf{x}}^2 - \frac{\mathbf{x}^2}{2m l^4} + \frac{(1+d)}{2m l^2} \right] \eta = \frac{1}{2m l^2} \eta^*. \quad (2.11)$$

Now we may verify, by inspection, that the solutions of Eq. (2.11) are of the form

$$\begin{aligned} \eta_{k_1 \dots k_d}(\mathbf{x} \cdot t) = & \left[\prod_{i=1}^d h_{k_i}(x_i/l) \right] \left[A_{k_1 \dots k_d} \exp(i\gamma_K \omega t/2\pi) \right. \\ & + [K^{1/2} + (K-1)^{1/2}]^2 \\ & \left. \times A_{k_1 \dots k_d}^* \exp(-i\gamma_K^* \omega t/2\pi) \right], \quad (2.12) \end{aligned}$$

where $A_{k_1 \dots k_d}$ is a complex constant, h_k is the normalized k th eigensolution of the unidimensional harmonic oscillator, the integer K is the sum

$$K = \sum_{i=1}^d k_i, \quad (2.13)$$

and the stability angles^{1,2} γ_K are given by

$$\gamma_K = \pm (2\pi/ml^2\omega)[K(K-1)]^{1/2}. \quad (2.14)$$

We observe that there are¹⁴

$$D(K, d) = (K+d-1)!/K!(d-1)! \quad (2.15)$$

configurations of the set $\{k_i\}$ that satisfies (2.13). Then, each γ_K has a degeneracy of order $D(K, d)$.

Since in the present case all stability angles are real numbers, we conclude that if a given fluctuation is infinitesimal at $t=0$, it will remain infinitesimal for any other time. So we say that the solutions of the type (2.6) are stable ones.

The stability angles (2.14) are the basic ingredients for implementing a WKB quantization of the model.^{1,2,7} This quantization will be presented in the next section.

From (2.14) we see that $\gamma_0 = \gamma_1 = 0$. γ_1 —having a degeneracy of degree d [see (2.15)]—is associated with the translational invariance of the theory, whereas γ_0 —which has no degeneracy—is the zero frequency mode correspondent to gauge invariance.

B. Confinement

Here the mechanism of confinement will be discussed in the context of the nonrelativistic logarithmic theory. The same phenomenon occurs in the relativistic theory, as shown in Ref. 13. For these logarithmic theories confinement happens to be a consequence of the nonexistence of the weak field limit.

Let us define the theory in a cubic box of volume L^d with periodic boundary conditions. L is such that $L \gg l, a, 1/m$, and later we will take the limit $L \rightarrow \infty$.

Consider a plane wave solution of Eq. (2.3)

$$\varphi_{\mathbf{k}, \omega}(\mathbf{x}, t) = A(\mathbf{k}, \omega) \exp[i(\mathbf{k}\mathbf{x} - \omega t)]. \quad (2.16)$$

From direct substitution of (2.14) into (2.3) we obtain the relation

$$\omega = (1/2m)[\mathbf{k}^2 - (1/l^2)\ln(|A|^2 a^d)]. \quad (2.17)$$

The energy associated with this solution will be

$$E(\mathbf{k}, A) = (|A|^2/2m)L^d[\mathbf{k}^2 - (1/l^2)[\ln(|A|^2 a^d) - 1]], \quad (2.18)$$

whereas the charge is

$$Q(A) = (|A|^2/2m)L^d. \quad (2.19)$$

From (2.15), (2.16), and (2.17) we get the following pair of relations involving ω, \mathbf{k}, E , and Q :

$$\omega(\mathbf{k}, Q) = \frac{1}{2m} \left\{ \mathbf{k}^2 - \frac{1}{l^2} \left[\ln \left(Q \left(\frac{a}{L} \right)^d \right) - 1 \right] \right\} \quad (2.20a)$$

and

$$E(\mathbf{k}, Q) = Q \left\{ \mathbf{k}^2 - \frac{1}{l^2} \left[\ln \left(Q \left(\frac{a}{L} \right)^d \right) - 1 \right] \right\}. \quad (2.20b)$$

Now, since \mathbf{k}^2 is always positive [otherwise $\varphi_{\mathbf{k}, \omega}$ will not be a solution of (2.3)], in the limit $L \rightarrow \infty$ we get

$$\omega(\mathbf{k}, Q) = \infty \quad \text{and} \quad E(\mathbf{k}, Q) = \infty. \quad (2.21)$$

This means that in the infinite volume limit we have no plane wave solutions for the classical version of the theory. We have no excitations around the vacuum ($\varphi = 0$). This is confinement. It follows from the fact that the Lagrangian (2.1) is nonanalytical in $|\varphi|^2$ when $|\varphi|^2 = 0$. It does not occur in any polynomial Lagrangian.

On the other hand we have seen that there exist excitations around the soliton (2.6). Obeying Eq. (2.11), these excitations are just linear superpositions of the solutions (2.12). The achievement is obvious: In the logarithmic theories, quantum fluctuations can manifest themselves only in the presence of a soliton that works as a bag for containing them.

We emphasize that the fluctuations (2.12) go to zero rapidly when any $|\chi_i|$ grows. This means that they are really confined within the soliton.

An interesting consequence of confinement is the fact that the set of stability angles is a discrete one. In theories where a continuum of stability angles exists, the sum over this continuum describes states of a soliton plus a certain amount of free elementary mesons coexisting.² In the present case the continuum does not exist since we have no free mesons.

In the relativistic version of the model the same mechanism occurs.¹³ There the equation for the fluctuations is also of the harmonic type. There are a large number of semiphenomenological papers in the literature where attempts are made to confine quarks by means of the harmonic oscillator potential—the trouble is that in those papers the potential is introduced by hand. It is remarkable that in the logarithmic theories we get the same picture starting from a local Lagrangian.

III. QUANTIZATION IN THE MANNER OF DHN

Here, in order to obtain the semiclassical energy spectrum we will use the DHN¹ formula as stated by Coleman.⁷ We leave to the next section the deduction of this spectrum by means of a canonical quantization procedure.

According to the DHN method the classical periods are “quantized” in the following way:

$$\int_0^T dt \int d^d \mathbf{x} \Pi_\omega(\mathbf{x}, t) \dot{\varphi}_\omega(\mathbf{x}, t) + \sum_{\gamma_i > 0} \left(n_i + \frac{D(\gamma_i)}{2} \right) \left(T \frac{d\gamma_i}{dT} - \gamma_i \right) = 2\pi N, \quad (3.1)$$

where $\varphi_\omega(\mathbf{x}, t)$ is the classical solution of period T ($\omega = 2\pi/T$), $\Pi_\omega(\mathbf{x}, t)$ is its conjugated momentum, $\{\gamma_i\}$ is the set of all stability angles, and $D(\gamma_i)$ is the degree of degeneracy of each stability angle. Any quantum state is characterized by an integer N and by the set $\{n_i; n_i = 0, 1, 2, \dots\}$. Solving Eq. (3.1) for the various states, we obtain a discrete set of values for the period: $T(N, n_1, n_2, \dots)$.

The allowed values of the energy are obtained from the expression⁷

$$E(N, n_1, n_2, \dots) = E_{\text{cl}}[T(N, n_1, n_2)] + \sum_{\gamma_i > 0} \left(n_i + \frac{D(\gamma_i)}{2} \right) \frac{d\gamma_i}{dT} \Big|_{T=T(N, n_1, n_2, \dots)}. \quad (3.2)$$

Here $E_{\text{cl}}^{(T)}$ is the classical energy of the soliton whose period is T . It is given by expression (2.4).

In our case, since $\Pi_\omega = i\varphi_\omega^\dagger$ [see Lagrangian (2.1)], the integral in (3.1) must be written as

$$\int_0^T dt \int d^d \mathbf{x} i\varphi_\omega^\dagger \dot{\varphi}_\omega. \quad (3.3)$$

From the fact that the stability angles of this model have a linear dependence on T [see (2.14)] we conclude that the sum \sum_{γ_i} in Eq. (3.1) is zero. So, our periods are quantized by the following expression:

$$\int_0^T dt \int d^d \mathbf{x} i\varphi_\omega^\dagger \dot{\varphi}_\omega = 2\pi N. \quad (3.4)$$

Evaluating explicitly the integral of expression (3.4), we get

$$(\pi^{1/2} l/a)^d \exp(d - 2ml^2\omega) = N. \quad (3.5)$$

This condition is equivalent to a quantization of the classical charge that is given in (2.9). The equivalence between semiclassical quantization and charge quantization was already pointed out in Refs. 15 and 16.

Using (3.5), the quantized values of ω are obtained:

$$\omega_N = (1/2ml^2)[d - \ln(a/\pi^{1/2}l)^d - \ln N]. \quad (3.6)$$

From (2.8) and (3.6) we conclude that the classical energy as function of N is given by

$$E_{\text{cl}}(N) = (N/2ml^2)[d + 1 - \ln(a/\pi^{1/2}l)^d - \ln N]. \quad (3.7)$$

In expression (2.15) we have the degree of degeneracy of each stability angle, whereas the stability angles themselves are shown in (2.14). Using them, one can write the sum \sum_{γ_i} that appears in (3.2) in the following manner:

$$\frac{1}{2ml^2} \sum_{K=0}^{\infty} \frac{(K+d-1)!}{K!(d-1)!} \sqrt{K(K-1)} + \frac{1}{ml^2} \sum_{K=0}^{\infty} n_K \sqrt{K(K-1)}. \quad (3.8)$$

The first sum in the above expression—which is clearly a divergent one—is the vacuum energy (note that it is independent of the particular state we are looking to), and so it will be dropped from the energy formula. Then, using (3.2), (3.7), and the finite part of (3.8), we get the spectrum

$$E(N; n_1, n_2, \dots) = (N/2ml^2)[d + 1 - \ln(a/\pi^{1/2}l)^d - \ln N] + (1/ml^2) \sum_{K=0}^{\infty} n_K \sqrt{K(K-1)}. \quad (3.9)$$

This is the WKB spectrum of the nonrelativistic logarithmic model in any number of space dimensions. Since in particular it holds for $d=3$, this is the first time—as far as we know—that a WKB quantization of a three-dimensional model has been done.

A. Zero-dimensional case

In zero dimension, K is always zero, since the set $\{k_1, k_2, \dots, k_d\}$ is an empty one. So, in this case the sum in (3.9) does not exist, and the spectrum can be written as

$$E_{d=0}(N) = (N/2ml^2)(1 - \ln N). \quad (3.10)$$

Now we will solve the zero-dimensional version of the logarithmic model in order to compare the exact spectrum with (3.10). Our conclusion will be that (3.10) is the exact spectrum.

When $d=0$, the Lagrangian is given by

$$L(a^*, a) = ia^* \dot{a} + (1/2ml^2)a^* a (\ln a^* a - 1). \quad (3.11)$$

From it one concludes that the canonical momentum associated with a is ia^* , whereas the Hamiltonian is

$$H(a^*, a) = (1/2ml^2)a^* a (1 - \ln a^* a). \quad (3.12)$$

It is well known that after imposing the canonical commutation relations

$$[a, ia^*] = i \quad \text{or} \quad [a, a^*] = 1, \quad (3.13)$$

the spectrum of a^*a is given by

$$Sp(a^*a) = 0, 1, 2, \dots, N, \dots. \quad (3.14)$$

So the spectrum of the Hamiltonian (3.12) will be just (3.10).

IV. CANONICAL QUANTIZATION

In this section we perform the canonical quantization of the model. Our procedure has much to do with those of Refs. 4, 5, and 6, even though some important differences must be stressed. In order to point out these differences, we shall start this section discussing the main ideas upon which our method is based.

The fields $\varphi(\mathbf{x}, t)$ and its momentum $\Pi(\mathbf{x}, t) = i\varphi^\dagger(\mathbf{x}, t)$ can—in a large variety of ways—be represented in terms of an infinite set of basic canonically conjugate pairs of operators $\{(a_0, b_0); (a_1, b_1); (a_2, b_2); \dots\}$. Let us consider the class of states $\{|a_0^n \dots\rangle\}$ — a_0^n being the n th eigenvalue of a_0 —where the eigenvalues of a_0^2 are very large when compared with the mean square values of the other basic operators (with the exception of b_0 , the momentum of a_0); i. e.,

$$(a_0^n)^2 \gg \langle a_0^n, \dots | a_i^2 | a_0^n, \dots \rangle \quad (4.1a)$$

$$(a_0^n)^2 \gg \langle a_0^n, \dots | b_i^2 | a_0^n, \dots \rangle \quad (4.1b)$$

for all $i \neq 0$.

When dealing with the mentioned class of states, it is natural to consider a_0 as a *leading operator* and to treat the other basic operators as fluctuations about it. So an approximate—and eventually soluble—Hamiltonian can be obtained by an expansion around a_0 retaining only terms up to second order in the nonleading operators. The following observations can serve as a brief outline of what we are going to do:

(i) In the present model the leading operator about which the Hamiltonian is expanded is the *charge operator*. So our approach is expected to hold only in the description of large charge states.

(ii) The representation that we choose for the fields is designed to satisfy the *semiclassical* canonical commutation relations

$$[\varphi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = i\delta(\mathbf{x} - \mathbf{y}) + O(1/\sqrt{a_0}). \quad (4.2)$$

Then, locality is guaranteed at least in a semiclassical sense.

(iii) Up to quadratic terms in the nonleading operators the Hamiltonian decouples into an infinite set of partial Hamiltonians, each of them depending only a given pair of basic canonically conjugate operators, i. e.,

$$H = H_0(a_0) + H_1(a_1, b_1) + H_2(a_2, b_2) + \dots + [\text{terms of order greater than 2 in } a_1, b_1; a_2, b_2; \text{etc.}] \quad (4.3)$$

The partial Hamiltonian H_0 is independent of b_0 (the momentum of a_0). Within the spirit of the approximation explained previously the terms of order greater than two in the fluctuations shall be dropped from the total Hamiltonian. Then the task of getting the spectrum becomes a very easy one because it suffices to sum up the energies of an infinite set of decoupled partial Hamiltonians.

We stress that our approach is different from the

usual semiclassical quantization methods, since instead of treating fluctuations around a classical field we do an expansion about a *leading operator*.

The Hamiltonian and the charge of the nonrelativistic logarithmic theory are—as we recall—given respectively by

$$H = \int d^d \mathbf{x} \left\{ \frac{1}{2m} \partial_{\mathbf{x}} \varphi^\dagger \partial_{\mathbf{x}} \varphi - \frac{1}{2m l^2} \varphi^\dagger \varphi [\ln(\varphi^\dagger \varphi a^d) - 1] \right\} \quad (4.4)$$

and

$$Q = \int d^d \mathbf{x} \varphi^\dagger \varphi. \quad (4.5)$$

Before exhibiting the basic operators and the field representation convenient for our case, we must introduce a complete set of functions of the coordinates. Being $\{k_1, k_2, \dots, k_d\}$ a set of d nonnegative integers, we define

$$F_{\{k_i\}}(\mathbf{x}) = \prod_{j=1}^d h_{k_j} \left(\frac{x_j}{l} \right), \quad (4.6)$$

where h_k is the k th normalized *real* wavefunction of the unidimensional harmonic oscillator. To some of these functions we give an abbreviated notation:

(a) The first one, where $k_j = 0$ for all j , we name $F_0(\mathbf{x})$, i. e.,

$$F_{\{0,0,\dots,0\}}(\mathbf{x}) = F_0(\mathbf{x}), \quad (4.7a)$$

and we recall that, since $F_0(\mathbf{x})$ is normalized, it will be

$$F_0(\mathbf{x}) = \left(\frac{1}{l \pi^{d/2}} \right)^{d/2} \exp \left(-\frac{\mathbf{x}^2}{2l^2} \right); \quad (4.7b)$$

(b) The functions (4.6) where $k_s = 1$ and $k_j = 0$ for all $j \neq s$ we name $F_s(\mathbf{x})$, i. e.,

$$F_{\{0 \dots k_s=1 \dots 0\}}(\mathbf{x}) = F_s(\mathbf{x}). \quad (4.8)$$

A. The basic operators

We will build fields with the following basic Hermitian operators:

(a) the pairs $(A(t), \theta(t))$ obeying the commutation relation

$$[A, \theta] = i; \quad (4.9)$$

(b) for each spatial direction s we define a pair of canonically conjugate operators $(\hat{z}_s(t), \hat{p}_s(t))$, whose commutation relations are

$$[\hat{z}_s, \hat{p}_s] = i\delta_{ss}, \quad (4.10a)$$

$$[\hat{z}_s, \hat{z}_s] = [\hat{p}_s, \hat{p}_s] = 0. \quad (4.10b)$$

From now on $\hat{z}(\hat{\mathbf{p}})$ will stand for a vector whose s th component is $\hat{z}_s(\hat{p}_s)$. Latter on we will interpret \hat{z} as the position of the center of mass of the particle described by a given state (collective coordinate⁴⁻⁶), whereas the eigenvalues of $\hat{\mathbf{p}}$ will be related to the momentum of that particle.

(c) for each set $\{k_i\}$, such that $K = \sum_{i=1}^d k_i > 1$ we also define a pair of canonically conjugate operators $(a_{\{k_i\}}(t), b_{\{k_i\}}(t))$. Their commutation relations are

$$[a_{\{k_i\}}, b_{\{k_i^*\}}] = i \delta_{\{k_i\} \{k_i^*\}} \\ = i \delta_{k_1} \delta_{k_2 k_2^*} \dots \delta_{k_d k_d^*}, \quad (4.11a)$$

$$[a_{\{k_i\}}, a_{\{k_i^*\}}] = [b_{\{k_i\}}, b_{\{k_i^*\}}] = 0. \quad (4.11b)$$

The remainder commutation relations among the basical operators are the following:

$$[A, \hat{z}_s] = [A, \hat{p}_s] = [A, a_{\{k_i\}}] = [A, b_{\{k_i\}}] = 0, \quad (4.12a)$$

$$[\theta, \hat{z}_s] = [\theta, \hat{p}_s] = [\theta, a_{\{k_i\}}] = [\theta, b_{\{k_i\}}] = 0, \quad (4.12b)$$

and

$$[\hat{z}_s, a_{\{k_i\}}] = [\hat{z}_s, b_{\{k_i\}}] = [\hat{p}_s, a_{\{k_i\}}] = [\hat{p}_s, b_{\{k_i\}}] = 0. \quad (4.12c)$$

B. The field representation

We are now in a position to present the field representation that will allow us to perform a WKB quantization of the model. In terms of the basical operators defined in the last subsection the field $\varphi(\mathbf{x}, t)$ will be written as¹⁷

$$\varphi(\mathbf{x}, t) = \exp(i\theta) \left[BF_0(\mathbf{x} - \hat{\mathbf{z}}) + \frac{i l}{2^{1/2}} \sum_{s=1}^d F_s(\mathbf{x} - \hat{\mathbf{z}}) \frac{\hat{p}_s}{A^{1/2}} \right. \\ \left. + \sum_{\{k_i, K>1\}} (a_{\{k_i\}} + i b_{\{k_i\}}) F_{\{k_i\}}(\mathbf{x} - \hat{\mathbf{z}}) \right], \quad (4.13)$$

where the operator B is given by

$$B = \left[A - \frac{l^2 \hat{\mathbf{p}}^2}{2A} - \sum_{\{k_i, K>1\}} (a_{\{k_i\}}^2 + b_{\{k_i\}}^2 - \frac{1}{2}) \right]^{1/2}. \quad (4.14)$$

Since the basical operators are Hermitian ones, the field $\varphi^\dagger(\mathbf{x}, t)$ must be

$$\varphi^\dagger(\mathbf{x}, t) = \left[BF_0(\mathbf{x} - \hat{\mathbf{z}}) - \frac{i l}{2^{1/2}} \sum_{s=1}^d \frac{\hat{p}_s}{A^{1/2}} F_s(\mathbf{x} - \hat{\mathbf{z}}) \right. \\ \left. + \sum_{\{k_i, K>1\}} (a_{\{k_i\}} - i b_{\{k_i\}}) F_{\{k_i\}}(\mathbf{x} - \hat{\mathbf{z}}) \right] \exp(-i\theta). \quad (4.15)$$

At this point it is appropriate to establish some connection between the operator approach developed here and other semiclassical methods of quantization.

As we shall see shortly, the operator A is just the charge. It is the leading operator about which the Hamiltonian will be expanded. We will consider only those states where the eigenvalue of A is very large (a more specific definition of what we mean by very large will be given latter on). This fact allows us to see the scheme outlined before in a different way:

Suppose that we remove the nonleading operators from the field representation (4.13), so defining what we call the leading part of the field $\varphi_L(\mathbf{x}, t)$:

$$\varphi_L(\mathbf{x}, t) = \exp(i\theta) A^{1/2} \left(\frac{1}{l\pi^{1/2}} \right)^{d/2} \exp \left[-\frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{2l^2} \right] \quad (4.16)$$

An expansion of any function of the fields about A is equivalent to an expansion around the leading field $\varphi_L(\mathbf{x}, t)$. But $\varphi_L(\mathbf{x}, t)$ —even though being an operator—has a remarkable resemblance with the classical soli-

ton (2.6) (a soliton whose center of mass position is $\hat{\mathbf{z}}$). In this sense we may say that the approximation which shall be done here is equivalent to an expansion of quantum fluctuation around the soliton itself.

C. Charge quantization

Since $\{F_0; F_s; F_{\{k_i\}}\}$ constitute an orthonormal basis, the charge operator Q defined in (4.5) will be

$$B^2 + \frac{l^2 \hat{\mathbf{p}}^2}{2A} + \sum_{\{k_i; K>1\}} \{a_{\{k_i\}}^2 + b_{\{k_i\}}^2 + i[a_{\{k_i\}}, b_{\{k_i\}}]\}. \quad (4.17)$$

Now using the commutation relations (4.9a) and the expression (4.14) for the operator B we conclude that

$$Q = A \quad (4.18)$$

as mentioned above. So the charge operator is the momentum conjugate to θ :

$$[Q, \theta] = i \quad \text{or} \quad Q = i \frac{\partial}{\partial \theta} \quad (4.19)$$

Then the eigenfunctions of Q must be of the form

$$\psi_q(\theta, c_i) = \exp(-i q \theta) R(c_i), \quad (4.20)$$

where q is the charge eigenvalue and c_i are others basical fields variables different from θ and Q .

Well, but θ is a cyclic variable; i. e., if we change θ into $\theta + 2n\pi$ (n being an integer), the field operators $\varphi(\mathbf{x}, t)$ and $\varphi^\dagger(\mathbf{x}, t)$ does not change [see (4.13) and (4.15)]. So, in order that the wavefunctional (4.20) be single valued in the space of field variables, it is necessary that the eigenvalues q be quantized in the following way

$$q_N = N, \quad (4.21)$$

where N is an integer. And since the charge operator Q is defined in (4.4) as the sum of nonnegative operators, N must be nonnegative.

D. The WKB approximation

Plugging the fields $\varphi(\mathbf{x}, t)$ and $\varphi^\dagger(\mathbf{x}, t)$ into the Hamiltonian (4.4) and performing the spatial integration, we obtain this Hamiltonian as a function of the operators Q (or A), $\hat{\mathbf{p}}$, $a_{\{k_i\}}$ and $b_{\{k_i\}}$.

Note that, since H does not depends on θ nor $\hat{\mathbf{z}}$, it commutes with Q and $\hat{\mathbf{p}}$.

Now we will explain what the WKB approximation is: Look first over the operators

$$R_{\{k_i\}} = a_{\{k_i\}}^2 + b_{\{k_i\}}^2 - \frac{1}{2}. \quad (4.22)$$

From the commutations relations (4.9a) we deduce that the eigenvalues of $R_{\{k_i\}}$ are nonnegative integers: $r_{\{k_i\}}$.

Let us consider the class of states $|N, \mathbf{p}, r_{\{k_i\}}\rangle^*$ (where \mathbf{p} is an eigenvalue of $\hat{\mathbf{p}}$) whose charge is very large when compared with $l^2 \hat{\mathbf{p}}^2$ and $\sum_{\{k_i; K>1\}} r_{\{k_i\}}$, i. e., states where

$$N \gg l^2 \hat{\mathbf{p}}^2 \quad (4.23a)$$

and

$$N \gg \sum_{\{k_i; K>1\}} r_{\{k_i\}}. \quad (4.23b)$$

Condition (4.23b) also implies that

$$N \gg \langle a_{\{k_i\}}^2 \rangle, \langle b_{\{k_i\}}^2 \rangle. \quad (4.24)$$

Then, in dealing with states that obey (4.23) (or linear combinations among them), we take Q to be the leading operators. The operators $\hat{\mathbf{p}}$, $a_{\{k_i\}}$, and $b_{\{k_i\}}$ are considered as small fluctuation about it. In this way we expand our Hamiltonian around Q retaining only terms up to second order in $\hat{\mathbf{p}}$, $a_{\{k_i\}}$, and $b_{\{k_i\}}$. This is the WKB approximation.

E. The expanded Hamiltonian

Due to the fact that Q commutes with $\hat{\mathbf{p}}$, $a_{\{k_i\}}$, and $b_{\{k_i\}}$, the above-mentioned expansion is unambiguous and easy to do. It is performed in Appendix A, and the resulting Hamiltonian is

$$H_0(Q) + H_1\left(\frac{\hat{\mathbf{p}}}{Q^{1/2}}\right) + \sum_{\{k_i; K>1\}} H_{\{k_i\}}(a_{\{k_i\}}, b_{\{k_i\}}), \quad (4.25)$$

where

$$H_0(Q) = \frac{1}{2ml^2} \left[d + 1 - \ln\left(\frac{a}{\pi^{1/2}l}\right)^d - \ln N \right], \quad (4.26)$$

the kinetic Hamiltonian $H_1(\hat{\mathbf{p}}/Q^{1/2})$ is given by

$$H_1\left(\frac{\hat{\mathbf{p}}}{Q^{1/2}}\right) = \frac{1}{2m} \frac{\hat{\mathbf{p}}^2}{Q} \quad (4.27)$$

and each one of the partial Hamiltonian $H_{\{k_i\}}$ is

$$H_{\{k_i\}} = \frac{1}{ml^2} [Kb_{\{k_i\}}^2 + (K-1)a_{\{k_i\}}^2] \quad (4.28)$$

We recall that $K = \sum_{i=1}^d k_i$.

The quantization of $H_0(Q)$ is trivial. Since we have seen above that the eigenvalues of the charge operator are $q_N = N$, the eigenvalues of $H_0(Q)$ must be

$$E_N = \frac{N}{2ml^2} \left[d + 1 - \ln\left(\frac{a}{\pi^{1/2}l}\right)^d - \ln N \right]. \quad (4.29)$$

The diagonalization of each one of the partial Hamiltonians $H_{\{k_i\}}$ is very simple. Due to the fact the coefficients of $a_{\{k_i\}}^2$ and $b_{\{k_i\}}^2$, in (4.28), are positive numbers, we recognize $H_{\{k_i\}}$ as the Hamiltonian of an harmonic oscillator. Then it has a discrete set of eigenvalues:

$$E_{n_{\{k_i\}}} = \frac{[K(K-1)]^{1/2}}{ml^2} n_{\{k_i\}} + \frac{1}{2} \frac{[K(K-1)]^{1/2}}{ml^2}, \quad (4.30)$$

where $n_{\{k_i\}}$ is an integer.

Being \mathbf{p} an eigenvalue of $\hat{\mathbf{p}}$, it is obvious that the eigenvalues of the kinetic Hamiltonian $H_1(\hat{\mathbf{p}}/Q^{1/2})$ are

$$E_N(\mathbf{p}) = (1/2mN)\mathbf{p}^2. \quad (4.31)$$

Then the spectrum of the total Hamiltonian (4.25) is given by

$$E(N, \mathbf{p}^2, n_{\{k_i\}}) = \frac{N}{2ml^2} \left[d + 1 - \ln\left(\frac{a}{\pi^{1/2}l}\right)^d - \ln N \right] + \sum_{\{k_i; K>1\}} \frac{[K(K-1)]^{1/2}}{ml^2} n_{\{k_i\}} + \sum_{\{k_i; K>1\}} \frac{1}{2} \frac{[K(K-1)]^{1/2}}{ml^2} + \frac{1}{2mN} \mathbf{p}^2. \quad (4.32)$$

The second sum in the above spectrum, the one independent from the state we are looking over, is the vacuum energy and can be dropped from the formula.

In order to compare the spectrum (4.32) with that obtained in Sec. III by using the DHN formula, it is convenient to define, for a given $K = \sum_{i=1}^d k_i$, the number

$$n_K = \sum_{\{k_i; \sum_{i=1}^d k_i = K\}} n_{\{k_i\}}. \quad (4.33)$$

So, in terms of n_K , after subtracting the vacuum energy, the spectrum (4.32) becomes

$$E(N, \mathbf{p}^2, n_{\{k_i\}}) = \frac{N}{2ml^2} \left[d + 1 - \ln\left(\frac{a}{\pi^{1/2}l}\right)^d - \ln N \right] + \sum_{K>1} \frac{[K(K-1)]^{1/2}}{ml^2} n_K + \frac{1}{2mN} \mathbf{p}^2. \quad (4.34)$$

When we take the value $\mathbf{p}^2 = 0$ in the above spectrum, it agrees with that given by Eq. (3.9).

F. The momentum operator

Now we will show more clearly the connection between the operator \hat{p}_s and the s th component of the momentum operator \hat{P}_s that is defined by

$$\hat{P}_s = - \int d^d \mathbf{x} \varphi^\dagger(\mathbf{x}, t) i \frac{\partial}{\partial x_s} \varphi(\mathbf{x}, t). \quad (4.35)$$

In Appendix B it is shown that

$$[\hat{z}_s, \hat{P}_{s'}] = i \delta_{ss'} + O(1/Q^{1/2}) \quad (4.36)$$

and

$$\hat{P}_s^2 = \hat{p}_s^2 + (\text{terms of third and fourth order in } \hat{p}_s, a_{\{k_i\}}, \text{ and } b_{\{k_i\}}). \quad (4.37)$$

From (4.36) we conclude that the semiclassical canonical commutation relations involving the c. m. position operator $\hat{\mathbf{z}}$ and the total momentum $\hat{\mathbf{P}}$ are preserved in this scheme of quantization.

In (4.37) the terms of third and fourth order in the nonleading operator can be neglected, since this procedure is in agreement with the approximation done for the Hamiltonian (see subsections D and E). Then the kinetic Hamiltonian H_1 can be written as

$$H_1 = (1/2mQ)\hat{\mathbf{P}}^2 \quad (4.38)$$

whereas its spectrum is

$$E_N(\mathbf{P}) = (1/2mN)\mathbf{P}^2, \quad (4.39)$$

where \mathbf{P} is an eigenvalue of the total momentum operator $\hat{\mathbf{P}}$.

G. Semiclassical locality

In order to complete our quantization scheme, we should say that the commutation relation among $\varphi(\mathbf{x}, t)$ and its canonical momentum $\Pi(\mathbf{x}, t)$ is given by

$$[\varphi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = i \cdot \delta(\mathbf{x} - \mathbf{y}) + O(1/Q^{1/2}). \quad (4.40)$$

This equation is deduced in Appendix C.

Then, when dealing with the class of states satisfying conditions (4.23a) and (4.23b), the term $O(1/Q^{1/2})$ can be dropped from Eq. (4.40), and we get a local theory. We recall that the mentioned class of states is just the one for which the spectrum has been obtained.

V. CONCLUSION

We succeeded in quantizing semiclassically the non-relativistic logarithmic model in any number of spatial dimension. Two methods of quantization were used: (a) Applying the DHN quantization formula, we were able to get the static spectrum of the model; (b) in Sec. IV a canonical quantization was done. There the charge was treated as a leading operator, and we expanded the Hamiltonian about it, retaining only terms up to second order in the nonleading operators. Doing so, besides the static spectrum we also obtained the kinetic part of the energy.

From this kinetic energy [see (4.34) or (4.39)] we conclude that a state of charge N is the nonrelativistic description of a particle, whose mass is

$$M_N = mN, \quad (5.1)$$

that can be interpreted as a bound state of N solitons of mass m .

The binding energy of this N solitons system is given by the static spectrum [see (3.9) or (4.34)]:

$$\begin{aligned} E(N, n_{\{k_i\}}) &= \frac{N}{2ml^2} \left[d + 1 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d - \ln N \right] \\ &+ \sum_{K>1} \frac{[K(K-1)]^{1/2}}{ml^2} n_K. \end{aligned} \quad (5.2)$$

Now let us briefly discuss the kind of "physical phenomena" that is described by the present model. Consider the theory defined by Lagrangian (2.1) when $d=3$ and

$$l \gg 1/m, \quad (5.3)$$

in this case, the states for which

$$N \lesssim (\pi^{1/2} l/a)^d \quad (5.4)$$

have a binding energy whose modulus is much smaller than the mass M_N . Then we are describing a sort of nonrelativistic "nuclear physics" of nonrotating particles.¹⁸

Unfortunately—since the model has no fundamental state—when N is sufficiently large the binding energy may be equal to (or greater than) the mass M_N , and the above picture fails.¹⁹

As a final remark we want to say that this method of considering the charge as the leading operator may—in principle—be applied to the semiclassical quantization of any theory invariant under gauge transformations of first kind and exhibiting solitons.

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APPENDIX A

In this appendix we do a Taylor series expansion of the Hamiltonian (4.4) about the charge operator Q up to second order in the nonleading operators. First of all this expansion is done about the operator B defined in Eq. (4.4). After this the operator B itself is expanded around Q .

Before proceeding a remark must be stated: It is known that due to the noncommutativity of the pairs of basic operators (in powers of which the Hamiltonian is developed) the mentioned expansion is not well defined. We have the freedom of ordering the operators that constitute a given term in various different ways. However—at least when we are concerned with approximations up to second order in the nonleading operators—each one of these various ways of ordering amounts only on a particular definition of what the vacuum energy is. Here for practical reasons our expansion will be guided by the following rule: The development of the Hamiltonian in Taylor series about the charge is done treating each one of the nonleading operators as c -numbers. Once the expansion is concluded they turn to be operators and the piece correspondent to the vacuum energy can be identified and subtracted.

In order to carry on the above mentioned expansion, it is convenient to introduce an auxiliary field $W(\mathbf{x}, t)$ that depends only upon the nonleading variables:

$$\begin{aligned} W(\mathbf{x}, t) &= \frac{i l}{2 l^2} \sum_{s=1}^d F_s(\mathbf{x} - \hat{z}) \frac{\hat{p}_s}{A^{1/2}} \\ &+ \sum_{\{k_i; K>1\}} (a_{\{k_i\}} + i b_{\{k_i\}}) F_{\{k_i\}}(\mathbf{x} - \hat{z}). \end{aligned} \quad (A1)$$

Note that $W(\mathbf{x}, t)$ is of first order in the nonleading operators and that it is orthogonal to $F_0(\mathbf{x} - \hat{z})$.

The fields $\varphi(\mathbf{x}, t)$ and $\varphi^\dagger(\mathbf{x}, t)$ are given by

$$\varphi(\mathbf{x}, t) = \exp(i\theta) [BF_0(\mathbf{x} - \hat{z}) + W(\mathbf{x}, t)] \quad (A2a)$$

and

$$\varphi^\dagger(\mathbf{x}, t) = [BF_0(\mathbf{x} - \hat{z}) + W^\dagger(\mathbf{x}, t)] \exp(-i\theta). \quad (A2b)$$

Let us look over the product $\varphi^\dagger(\mathbf{x}, t)\varphi(\mathbf{x}, t)$ that is a basic ingredient to construct the Hamiltonian:

$$\begin{aligned} \varphi^\dagger(\mathbf{x}, t)\varphi(\mathbf{x}, t) &= B^2 F_0^2(\mathbf{x} - \hat{z}) + W^\dagger(\mathbf{x}, t)W(\mathbf{x}, t) \\ &+ [BF_0(\mathbf{x} - \hat{z})W(\mathbf{x}, t) + W^\dagger(\mathbf{x}, t)F_0(\mathbf{x} - \hat{z})]. \end{aligned} \quad (A3)$$

We are interested in the following function of the fields:

$$T(\mathbf{x}, t) = \varphi^\dagger \varphi [\ln(\varphi^\dagger \varphi a^d) - 1]. \quad (A4)$$

Then we expand $T(\mathbf{x}, t)$ about the dominant operator $B^2 F_0^2(\mathbf{x} - \hat{z})$ going up to second order in $W(\mathbf{x}, t)$ (that is equivalent to second order in the nonleading operators). We recall that at this step of the calculations the nonleading operators are treated as c -numbers. So $T(\mathbf{x}, t)$ can be written as

$$T(\mathbf{x}, t) = t_0 + t_1 + t_2 + [\text{terms of order greater than 2 on } W(\mathbf{x}, t)], \quad (A5)$$

where

$$t_0 = B^2 F_0^2 [\ln(B^2 F_0^2 a^d) - 1], \quad (\text{A6a})$$

$$t_1 = \ln(B^2 F_0^2 a^d) B F_0 (W^\dagger + W), \quad (\text{A6b})$$

and

$$t_3 = [\ln(B^2 F_0^2 a^d) + 1] W^\dagger W + \frac{1}{2} [(W^\dagger)^2 + W^2]. \quad (\text{A6c})$$

The other product of interest to compute the Hamiltonian is $\partial_{\mathbf{x}} \varphi^\dagger \partial_{\mathbf{x}} \varphi$. It can be written as

$$\begin{aligned} \partial_{\mathbf{x}} \varphi^\dagger \partial_{\mathbf{x}} \varphi &= \partial_{\mathbf{x}} (B F_0) \partial_{\mathbf{x}} (B F_0) + \partial_{\mathbf{x}} W^\dagger \partial_{\mathbf{x}} W \\ &\quad + \partial_{\mathbf{x}} (B F_0) \partial_{\mathbf{x}} W + \partial_{\mathbf{x}} W^\dagger \partial_{\mathbf{x}} (B F_0). \end{aligned} \quad (\text{A7})$$

From (A4), (A5), (A6), and (A7) one concludes that the Hamiltonian (4.4) may be represented by

$$\begin{aligned} H &= H_I + H_{II} + H_{III} \\ &\quad + [\text{terms of order greater than 2 in the nonleading operators}], \end{aligned} \quad (\text{A8})$$

where

$$\begin{aligned} H_I &= \int d^d \mathbf{x} \left\{ \frac{1}{2m} \partial_{\mathbf{x}} (B F_0) \partial_{\mathbf{x}} (B F_0) + \frac{1}{2m l^2} \right. \\ &\quad \left. \times [1 - \ln(B^2 F_0^2 a^d)] B^2 F_0^2 \right\}, \end{aligned} \quad (\text{A9a})$$

$$\begin{aligned} H_{II} &= \int d^d \mathbf{x} \left\{ \frac{1}{2m} [\partial_{\mathbf{x}} (B F_0) \partial_{\mathbf{x}} W + \partial_{\mathbf{x}} W^\dagger \partial_{\mathbf{x}} (B F_0)] \right. \\ &\quad \left. - \frac{1}{2m l^2} \ln(B^2 F_0^2 a^d) B F_0 (W^\dagger + W) \right\}, \end{aligned} \quad (\text{A9b})$$

and

$$\begin{aligned} H_{III} &= \int d^d \mathbf{x} \left\{ \frac{1}{2m} \partial_{\mathbf{x}} W^\dagger \partial_{\mathbf{x}} W - \frac{1}{2m l^2} [\ln(B^2 F_0^2 a^d) + 1] W^\dagger W \right. \\ &\quad \left. - \frac{1}{2m l^2} \frac{1}{2} [(W^\dagger)^2 + W^2] \right\}. \end{aligned} \quad (\text{A9c})$$

Now we recall that

$$F_0(\mathbf{x} - \hat{\mathbf{z}}) = \left(\frac{1}{l \pi^{1/2} l} \right)^{d/2} \exp \left[- \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{2 l^2} \right], \quad (\text{A10})$$

and in consequence of this we get

$$\ln(B^2 F_0^2 a^d) = \ln B^2 + \ln \left(\frac{a}{\pi^{1/2} l} \right)^d - \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2}. \quad (\text{A11})$$

Integrating by parts the terms having derivatives in Eqs. (A9), and using (A10) and (A11), one obtains

$$\begin{aligned} H_I &= \frac{B^2}{2m l^2} \int d^d \mathbf{x} F_0(\mathbf{x} - \hat{\mathbf{z}}) \left[- l^2 \partial_{\mathbf{x}}^2 + \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2} \right. \\ &\quad \left. + 1 - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] F_0(\mathbf{x} - \hat{\mathbf{z}}), \end{aligned} \quad (\text{A12a})$$

$$\begin{aligned} H_{II} &= \frac{B}{2m l^2} \int d^d \mathbf{x} (W^\dagger + W) \left[- l^2 \partial_{\mathbf{x}}^2 + \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2} \right. \\ &\quad \left. - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] F_0(\mathbf{x} - \hat{\mathbf{z}}), \end{aligned} \quad (\text{A12b})$$

and

$$\begin{aligned} H_{III} &= \frac{1}{2m l^2} \int d^d \mathbf{x} W^\dagger \left[- l^2 \partial_{\mathbf{x}}^2 + \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2} - \ln B^2 \right. \\ &\quad \left. - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d - 1 \right] W - \frac{1}{2} [(W^\dagger)^2 + W^2]. \end{aligned} \quad (\text{A12c})$$

From the definition of $F_0(\mathbf{x})$ given in Sec. IV [see (4.6) and (4.7a)] we have

$$\left[- l^2 \partial_{\mathbf{x}}^2 + \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2} \right] F_0(\mathbf{x} - \hat{\mathbf{z}}) = d F_0(\mathbf{x} - \hat{\mathbf{z}}). \quad (\text{A13})$$

Putting (A13) into (A12a) and (A12b), we see that H_I and H_{II} are

$$\begin{aligned} H_I &= \frac{B^2}{2m l^2} \left[d + 1 - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] \\ &\quad \times \int d^d \mathbf{x} [F_0(\mathbf{x} - \hat{\mathbf{z}})]^2 \end{aligned} \quad (\text{A14a})$$

and

$$\begin{aligned} H_{II} &= \frac{B^2}{2m l^2} \left[d - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] \\ &\quad \times \int d^d \mathbf{x} (W^\dagger + W) F_0(\mathbf{x} - \hat{\mathbf{z}}) \end{aligned} \quad (\text{A14b})$$

Since, by construction, $F_0(\mathbf{x})$ is normalized and $W(\mathbf{x}, t)$ is orthogonal to $F_0(\mathbf{x} - \hat{\mathbf{z}})$ [see (A1)], it follows that

$$H_I = \frac{B^2}{2m l^2} \left[d + 1 - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] \quad (\text{A15a})$$

and

$$H_{II} = 0. \quad (\text{A15b})$$

In order to obtain H_{III} , one must substitute $W(\mathbf{x}, t)$ given by Eq. (A1) into (A12c). Considering that $\{F_{\{k_i\}}\}$ constitutes an orthonormal set and that [see (4.6) and (4.7b)]

$$\left[- l^2 \partial_{\mathbf{x}}^2 + \frac{(\mathbf{x} - \hat{\mathbf{z}})^2}{l^2} \right] F_{\{k_i\}}(\mathbf{x} - \hat{\mathbf{z}}) = (2K + d) F_{\{k_i\}}(\mathbf{x} - \hat{\mathbf{z}}), \quad (\text{A16})$$

one gets (we recall that $A = Q$)

$$\begin{aligned} H_{III} &= \frac{1}{4m Q} \left[2 + d - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] \sum_{s=1}^d \hat{p}_s^2 \\ &\quad + \frac{1}{2m l^2} \sum_{\{k_i; iK > 1\}} \left\{ \left[2K + d - 1 - \ln B^2 - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right] \right. \\ &\quad \left. \times (a_{\{k_i\}} - i b_{\{k_i\}})(a_{\{k_i\}} + i b_{\{k_i\}}) + a_{\{k_i\}}^2 - b_{\{k_i\}}^2 \right\}. \end{aligned} \quad (\text{A17})$$

Now, expanding H_I given by (A15a) about the charge operator, one sees that [B is given by (4.14)]

$$\begin{aligned} H_I &= \frac{Q}{2m l^2} \left(d + 1 - \ln Q - \ln \left(\frac{a}{\pi^{1/2} l} \right)^d \right) \\ &\quad + \frac{1}{4m Q} \left[\ln Q + \ln \left(\frac{a}{\pi^{1/2} l} \right)^d - d \right] \sum_{s=1}^d \hat{p}_s^2 \\ &\quad + \frac{1}{2m l^2} \left[\ln Q + \ln \left(\frac{a}{\pi^{1/2} l} \right)^d - d \right] \\ &\quad \times \sum_{\{k_i; iK > 1\}} (a_{\{k_i\}}^2 + b_{\{k_i\}}^2 - \frac{1}{2}) \\ &\quad + [\text{terms in order greater than 2 in the nonleading operator}]. \end{aligned} \quad (\text{A18})$$

Then summing (A15b), (A17), and (A18), we conclude that the total Hamiltonian (A8) is just that written in expression (4.25).

APPENDIX B

Without loss of generality we will deduce Eqs. (4.36) and (4.37) in the *one-dimensional* theory. There the momentum operator is

$$\hat{P} = -i \int dx \varphi^\dagger \frac{\partial}{\partial x} \varphi$$

$$= \frac{-i}{l^2} \int dx \left[\sum_{K=0}^{\infty} \beta_K^* h_K(\xi) \right] \left[\sum_{K'=0}^{\infty} \beta_{K'} h_{K'}(\xi) \right], \quad (\text{B1})$$

where

$$\xi = (x - \hat{z})/l, \quad \beta_0 = B, \quad \beta_1 = i\hat{p}/(2A)^{1/2}, \quad \text{and}$$

(when $K > 1$) $\beta_K = a_K + ib_K$.

Then \hat{P} can be written as

$$\hat{P} = \frac{-i}{l} \sum_{K=0}^{\infty} \sum_{K'=0}^{\infty} \beta_K^* \beta_{K'} \int d\xi h_K(\xi) \frac{\partial}{\partial \xi} h_{K'}(\xi). \quad (\text{B2})$$

Since h_K is the K th eigenfunction of the harmonic oscillator, the integral in (B2) gives

$$d\xi h_K(\xi) \frac{\partial}{\partial \xi} h_{K'}(\xi) = \frac{1}{2^{1/2} l} [(K+1)^{1/2} \delta_{K+1, K'} - K^{1/2} \delta_{K-1, K'}]. \quad (\text{B3})$$

From (B2) one concludes that \hat{P} will be

$$\hat{P} = \frac{-i}{l} \sum_{K=0}^{\infty} \frac{1}{2^{1/2} l} [(K+1)^{1/2} \beta_K^* \beta_{K+1} - K^{1/2} \beta_K^* \beta_{K-1}]. \quad (\text{B4})$$

Using the definitions of β_K that were given just below Eq. (B1), one obtains

$$\hat{P} = \frac{B}{A^{1/2} l} \hat{p} - 2^{1/2} l \frac{\hat{p}}{A^{1/2} l} a_2 + \frac{2^{1/2}}{l} \sum_{K=2}^{\infty} (K+1)^{1/2} (a_K b_{K+1} - b_K a_{K+1}). \quad (\text{B5})$$

From expression (4.14) one deduces that

$$B/A^{1/2} = 1 + O(1/A^{1/2}) \quad (\text{B6})$$

and

$$(B/A^{1/2})^2 \hat{p}^2 = \hat{p}^2 + [\text{terms in fourth order in the nonleading operators}]. \quad (\text{B7})$$

Finally using (B5), (B6), (B7), and the commutation relation (4.10a) one concludes that (4.36) and (4.37) hold.

APPENDIX C

Here we will compute the commutator

$$(1/i)[\varphi(\mathbf{x}, t), \Pi(\mathbf{y}, t)] = [\varphi(\mathbf{x}, t), \varphi^\dagger(\mathbf{y}, t)]. \quad (\text{C1})$$

First of all let us recall that the commutation relations (4.9), (4.10), (4.11), and (4.12) demands that

$$\exp(i\theta)G(A) \exp(-i\theta) = G(A+1) \quad (\text{C2})$$

[for any function $G(A)$] and

$$[\hat{p}_s, F_0(\xi)] = \frac{-i}{l^2} F_s(\xi) \quad (\text{C3})$$

where $\xi = \mathbf{x} - \hat{z}$.

Using Eqs. (4.13) and (4.15), we conclude that the

commutator (C1) is given by the following sum:

$$\alpha + \sum_s \alpha_s + \sum_{s, s'} \alpha_{ss'} + \sum_{\{k_i; K > 1\}} \alpha_{\{k_i\}} \quad (\text{C4})$$

$$+ \sum_{s, \{k_i; K > 1\}} \alpha_{s\{k_i\}} + \sum_{\substack{\{k_i; K > 1\} \\ \{k'_i; K > 1\}}} \alpha_{\{k_i\}\{k'_i\}}$$

whose components are (from now on $\xi = \mathbf{x} - \hat{z}$ and $\rho = \mathbf{y} - \hat{z}$,

$$\alpha = [\exp(i\theta)BF_0(\xi), BF_0(\rho) \exp(-i\theta)], \quad (\text{C5a})$$

$$\alpha_s = [\exp(i\theta)BF_0(\xi), -il(\hat{p}_s/A^{1/2})F_s(\rho) \exp(-i\theta)] + [\exp(i\theta)F_s(\xi)il(\hat{p}_s/A^{1/2}), BF_0(\rho) \exp(-i\theta)], \quad (\text{C5b})$$

$$\alpha_{ss'} = [\exp(i\theta)F_s(\xi)il(\hat{p}_s/A^{1/2}), -il(\hat{p}_{s'}/A^{1/2})F_{s'}(\rho) \exp(-i\theta)], \quad (\text{C5c})$$

$$\alpha_{\{k_i\}} = [\exp(i\theta)BF_0(\xi), (a_{\{k_i\}} - ib_{\{k_i\}})F_{\{k_i\}}(\rho) \exp(-i\theta)] + [\exp(i\theta)(a_{\{k_i\}} + ib_{\{k_i\}})F_{\{k_i\}}(\xi), BF_0(\rho) \exp(-i\theta)], \quad (\text{C5d})$$

$$\alpha_{s\{k_i\}} = [\exp(i\theta)F_s(\xi)il(\hat{p}_s/A^{1/2}), (a_{\{k_i\}} - ib_{\{k_i\}}) \times F_{\{k_i\}}(\rho) \exp(-i\theta)] + [\exp(i\theta)a_{\{k_i\}} + ib_{\{k_i\}})F_{\{k_i\}}(\xi), -il(\hat{p}_s/A^{1/2})F_s(\rho) \exp(-i\theta)], \quad (\text{C5e})$$

and finally

$$\alpha_{\{k_i\}\{k'_i\}} = [\exp(i\theta)(a_{\{k_i\}} + ib_{\{k_i\}})F_{\{k_i\}}(\xi), (a_{\{k'_i\}} - ib_{\{k'_i\}}) \times F_{\{k'_i\}}(\rho) \exp(-i\theta)]. \quad (\text{C5f})$$

Now let us obtain each one of the α terms. The first one is

$$\alpha = [\exp(i\theta)B^2(A) \exp(-i\theta) - B^2(A)]F_0(\xi)F_0(\rho). \quad (\text{C6})$$

Using (C2), we get

$$\alpha = [B^2(A+1) - B^2(A)]F_0(\xi)F_0(\rho), \quad (\text{C7})$$

where the operator $B(A)$ is given in (4.14). Then

$$\alpha = \left[1 + \frac{l^2}{2} \frac{\hat{p}^2}{A(A+1)} \right] F_0(\xi)F_0(\rho), \quad (\text{C8a})$$

or

$$\alpha = F_0(\xi)F_0(\rho) + O(1/A^2). \quad (\text{C8b})$$

The terms α_s are

$$\alpha_s = (-il/2^{1/2}) \{ \exp(i\theta)BF_0(\xi)(\hat{p}_s/A^{1/2})F_s(\rho) \exp(-i\theta) - (\hat{p}_s/A^{1/2})F_s(\rho)BF_0(\xi) + \exp(i\theta)F_s(\xi)(\hat{p}_s/A^{1/2})BF_0(\rho) \exp(-i\theta) - BF_0(\rho)F_s(\xi)(\hat{p}_s/A^{1/2}) \}$$

$$= (-il/2^{1/2}) \{ F_0(\xi)\hat{p}_sF_s(\rho) - \hat{p}_sF_s(\rho)F_0(\xi) + F_s(\xi)\hat{p}_sF_0(\rho) - F_0(\rho)F_s(\xi)\hat{p}_s \} + O(1/A). \quad (\text{C9})$$

From (C3) and (C9) it follows that

$$\alpha_s = F_s(\xi)F_s(\rho) + O(1/A). \quad (\text{C10})$$

The other relevant terms are

$$\begin{aligned} \alpha_{\{k_i\}\{k_i^*\}} &= [a_{\{k_i\}} + ib_{\{k_i\}}, a_{\{k_i^*\}} - ib_{\{k_i^*\}}] F_{\{k_i\}}(\xi) F_{\{k_i^*\}}(\rho) \\ &= \delta [b_{\{k_i\}}, a_{\{k_i^*\}}] - [a_{\{k_i\}}, b_{\{k_i^*\}}] F_{\{k_i\}}(\xi) F_{\{k_i^*\}}(\rho). \end{aligned} \quad (C11)$$

From (4.11) one concludes that

$$\alpha_{\{k_i\}\{k_i^*\}} = \delta_{\{k_i\}\{k_i^*\}} F_{\{k_i\}}(\xi) F_{\{k_i^*\}}(\rho). \quad (C12)$$

The remainder terms (α_{ss^*} , $\alpha_{\{k_i\}}$, and $\alpha_{s\{k_i\}}$) are not relevant in the context of our semiclassical approximation. α_{ss^*} and $\alpha_{s\{k_i\}}$ are obviously given by

$$\alpha_{ss^*} = O(1/A) \quad (C13)$$

and

$$\alpha_{s\{k_i\}} = O(1/A^{1/2}), \quad (C14)$$

whereas $\alpha_{\{k_i\}}$ can be written as

$$\begin{aligned} \alpha_{\{k_i\}} &= [\exp(i\theta)B \exp(-i\theta) - B] (a_{\{k_i\}} - ib_{\{k_i\}}) F_0(\xi) F_{\{k_i\}}(\rho) \\ &\quad + [B - \exp(i\theta)B \exp(-i\theta)] (a_{\{k_i\}} + ib_{\{k_i\}}) F_0(\rho) F_{\{k_i\}}(\xi). \end{aligned} \quad (C15)$$

Using (C2) and the expression for $B(A)$, it is clear that

$$\alpha_{\{k_i\}} = O(1/A^{1/2}) \quad (C16)$$

Then the commutation relation (C1) [that is, the sum (C4)] can be written as [see (C8), (C10), (C12)–(C14), and (C16)]

$$\begin{aligned} F_0(\xi) F_0(\rho) + \sum_s F_s(\xi) F_s(\rho) \\ + \sum_{\substack{\{k_i, k_i^*\} \\ \{k_i^*, k_i\}}} \delta_{\{k_i\}\{k_i^*\}} F_{\{k_i\}}(\xi) F_{\{k_i^*\}}(\rho). \end{aligned} \quad (C17)$$

Taking in account the fact that $\xi = \mathbf{x} - \hat{\mathbf{z}}$ and $\rho = \mathbf{y} - \hat{\mathbf{z}}$ it follows that

$$\begin{aligned} [\varphi(\mathbf{x}, t), \varphi^\dagger(\mathbf{y}, t)] \\ = F_0(\mathbf{x} - \hat{\mathbf{z}}) F_0(\mathbf{y} - \hat{\mathbf{z}}) \\ + \sum_s F_s(\mathbf{x} - \hat{\mathbf{z}}) F_s(\mathbf{y} - \hat{\mathbf{z}}) + \sum_{\{k_i\}} F_{\{k_i\}}(\mathbf{x} - \hat{\mathbf{z}}) F_{\{k_i\}}(\mathbf{y} - \hat{\mathbf{z}}) \\ + O(1/A^{1/2}). \end{aligned} \quad (C18)$$

And since $\{F_0, F_s, F_{\{k_i\}}\}$ is a complete orthonormal basis, we obtain expression (4.40):

$$[\varphi(\mathbf{x}, t), \varphi^\dagger(\mathbf{y}, t)] = \delta(\mathbf{x} - \mathbf{y}) + O(1/A^{1/2}). \quad (C19)$$

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¹⁸It is very easy to verify that rotating solitons may be obtained in logarithmic theories with a more complex internal symmetry. For instance, if we start—in three dimensions—with a four-component field in Lagrangian (2.1), we shall get solitons having angular momentum.

¹⁹This difficulty can eventually be remedied if we couple the field $\varphi(\mathbf{x}, t)$ to the electromagnetic field. Doing so, the model could gain a fundamental state because each particle of charge N will acquire a positive electromagnetic energy that grows with N and can, in principle, cancel out the negative part of the original spectrum in the large N limit.

Lorentz-type internal symmetry

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An internal symmetry, which is based on a generalization of SU(3) in analogy to the external Poincaré group, is proposed for elementary particles. The so-called exact symmetry limit is assumed to be valid in some intrinsic "rest frame," while the symmetry breaking is geometrically obtained by leaving this frame by some defined SU(3) boosts. The baryon number, which SU(3) does not fix for a given representation, can be defined here in analogy to the ordinary helicity. Thus it can be used to characterize some restricted SU(3) representations which provide the basis for a generalized quark model. Two kinds of quarks exist in the theory: the conventional ones and pseudoquarks possessing unexpected leptonic-like properties. For the quarks of the first kind strong currents are constructed and a strong interaction model, built as local couplings of those currents, is also presented. The model is consistent with dual quark diagrams and contains a mathematical mechanism by which n quarks and \bar{n} antiquarks enter an interaction vertex only if $n - \bar{n} \equiv 0 \pmod{3}$. Finally the mass operator is discussed in the light of the proposed symmetry.

I. INTRODUCTION

From its very beginning internal symmetry for elementary particles was introduced as a broken one. Nevertheless, the concept of an exact symmetry limit is very popular, and even particle states are still classified (without solid justification) according to the irreducible representations of the exact symmetry. Several attempts have been made to generalize the SU(3) internal symmetry, most of them by considering higher SU(n) symmetries,¹⁻³ but from the symmetry breaking point of view nothing has been changed. Here we present a nonconventional approach to symmetry breaking. We propose an internal symmetry group built in a natural analogy to the Poincaré group, the only continuous symmetry group which is physically exact. We call this new symmetry group: the hyper-Poincaré group, and we use similar notations. However, we emphasize that *the real Lorentz group appears here only as a mathematical analog*, and all the quantities involved are intrinsic. Moreover, in this paper, no attempt is made to look for possible connections⁴ between the internal and the external spaces. Confrontation with known "no-go" theorems⁵ is thereby avoided.

The proposed symmetry group is a group of transformations acting in a special nine-dimensional space, where it is somewhat surprising to find a *third-order metric tensor* $g_{\mu\nu\lambda}$ whose mathematical properties dominate the theory. These transformations include a homogeneous part, built of eight rotations and eight boosts generating a nonchiral SU(3) × SU(3) algebra, as well as of nine translations which complete the inhomogeneous part. The group contains three invariants: M^3 , $M^3 C_2$, $M^3 C_3$, where M^3 is the intrinsic analog of the Lorentzian m^2 , and C_2 , C_3 are the SU(3) Casimir operators whose values are determined in some generalized intrinsic "rest frame." The little group in this frame turns out to be the usual SU(3), a property which forces us to relate it to the exact symmetry limit mentioned before. Leaving this frame by some boost introduces symmetry breaking similar

to a broken rotational symmetry, since the generators of the little group are no longer pure rotations⁶; *the symmetry breaking is thus of geometrical origin.*⁷

Physical difficulties connected with $M^3 \neq 0$ lead us to assume that only representations belonging to the $M=0$ case have particle interpretation. The dramatic consequence of such an assumption is the spontaneous appearance of the missing baryon number. This quantity, which is undetermined within SU(3), is now defined in a complete analogy to the ordinary helicity. That is a component of the F spin along the hypermomentum direction which satisfies $B(3) = \frac{1}{3}$ and $B(3^*) = -\frac{1}{3}$. It is an invariant only when $M=0$, and therefore it can be used to characterize the representations only in this case. The representations associated with $M=0$ are not as familiar as the ordinary ones because the algebra generated by the little-group generators is no longer semisimple. The limitations imposed on these representations lead to the result that the quark model is the only choice which does not prevent the population of the physical known SU(3) multiplets. In Sec. IV the existence of two entirely independent classes of representations is shown, leading to two different types of quarks. The quarks of the first kind are the conventional ones, but those of the second kind, called pseudoquarks, possess new properties. Such objects are characterized by only one diagonal (Q) generator [an unexpected property when the underlying symmetry is SU(3)]; they are a d - s mixture⁸ and can exist in two different versions. These are leptonic-like properties which are found in an SU(3)-based theory.

In Sec. V a model of quark interactions is introduced, based on some fundamental mathematical properties of the algebraic structure of the theory. We propose a strong interaction model, built as local couplings of covariant and contravariant independent quark currents, *which allow n quarks and \bar{n} antiquarks of the first kind to enter an interaction vertex only if $n - \bar{n} \equiv 0 \pmod{3}$* . We further adopt the "classical" assumption that any physical particle is a bound state of the interacting quarks, and hence we get a mathematical mechanism which explains why the low-lying states are of triality zero. This model has general features of a dual quark

^{a)}Work in partial fulfillment of the requirements for the D. Sc. degree.

model because the current structure (quark creation and annihilation) contains the element of quark-line conservation.

At the end of this paper we discuss qualitatively possible mass operators from the proposed symmetry point of view. We attempt to explain why such a quadratic operators (m^2) cannot be a hyper-Lorentz scalar, which is cubic, and why in our opinion it can be some zero component of a tensor. In such a way the mass operator will be a rotational invariant only in the "rest frame" (the exact symmetry limit), and any boost will destroy this partial invariance.

II. THE HYPER-POINCARÉ TRANSFORMATION

Let x^μ be a 9-vector and X its associated matrix given by $X = x^\mu \lambda_\mu = \sqrt{\frac{2}{3}} x^0 I + \mathbf{x} \cdot \boldsymbol{\lambda}$, where λ are Gell-Mann's matrices and I is the identity. If the determinant of X ,

$$\det X = \frac{2\sqrt{2}}{3} g_{\mu\nu\lambda} x^\mu x^\nu x^\lambda, \quad (1)$$

is invariant under $X \rightarrow X' = AXA^\dagger$, then we are left with a 16-parameter transformation matrix A , such that $|\det A| = 1$. The coefficients $g_{\mu\nu\lambda}$ form a symmetric third-order metric tensor. It is given explicitly by

$$\begin{aligned} g_{000} &= 1/\sqrt{3}, \quad g_{i00} = 0, \\ g_{ij0} &= -(1/2\sqrt{3})\delta_{ij}, \quad g_{ijk} = (1/\sqrt{2})d_{ijk}, \end{aligned} \quad (2)$$

where δ_{ij} , d_{ijk} are the familiar SU(3) symmetric structure constants, and the notation is

$$\begin{aligned} \mu, \nu, \lambda &= 0, 1, \dots, 8, \\ i, j, k &= 1, \dots, 8. \end{aligned}$$

The normalization of this metric tensor is

$$g^{\mu\alpha\beta} g_{\nu\alpha\beta} = \delta^\mu_\nu. \quad (3)$$

The hyper-Lorentz transformation R is now defined by $x \rightarrow x' = Rx$, such that

$$g_{\alpha\beta\gamma} R^\alpha_\mu R^\beta_\nu R^\gamma_\sigma = g_{\mu\nu\sigma}. \quad (4)$$

Among the various transformation families satisfying (4), we are concerned only with those related to A . One finds the connection $R^\mu_\nu = \frac{1}{2} \text{Tr}(\lambda_\mu A \lambda_\nu A^\dagger)$, so that $A \rightarrow R(A)$ is a homomorphism of $SL(3, C)$ onto this restricted hyper-Lorentz group. These special R 's have the expected "proper orthochronous Lorentzian" properties: $R^0_0 \geq 1$ and $\det R = +1$.

Next we consider the infinitesimal transformation which is of the form: $R \approx I + \omega$. As a consequence of (4), ω must obey the equation

$$g_{\mu\nu\alpha} \omega^\alpha_\lambda + g_{\mu\alpha\lambda} \omega^\alpha_\nu + g_{\alpha\nu\lambda} \omega^\alpha_\mu = 0, \quad (5)$$

and by the more interesting part

$$\begin{bmatrix} x'^0 \\ x'^3 \\ x'^8 \end{bmatrix} = \begin{bmatrix} \frac{1}{3}(e^{-2B} + 2e^B \cdot \cosh A); & \sqrt{\frac{2}{3}} e^B \cdot \sinh A; \\ \sqrt{\frac{2}{3}} e^B \cdot \sinh A; & e^B \cdot \cosh A; \\ (\sqrt{2}/3)(e^B \cdot \cosh A - e^{-2B}); & \sqrt{\frac{2}{3}} e^B \cdot \sinh A; \end{bmatrix} \cdot \begin{bmatrix} x^0 \\ x^3 \\ x^8 \end{bmatrix} \quad (9b)$$

whose solution

$$\begin{aligned} \omega^0_0 &= 0, \\ \omega^i_0 &= \omega^0_i = \sqrt{\frac{2}{3}} \beta_i, \\ \omega^i_j &= f_{ijk} \alpha_k + d_{ijk} \beta_k, \end{aligned} \quad (6)$$

consists of 16 parameters grouped into two classes. The α are identified as the known SU(3) rotation parameters, while the β are the added boost parameters. The corresponding unitary operator U is of the form:

$$U(I + \omega) = I + iF^\nu_{\cdot\mu} \omega^\mu_\nu = I + i\alpha \cdot \mathbf{F} + i\beta \cdot \mathbf{B}. \quad (7)$$

Making use of the group property $U(R_2)U(R_1) = U(R_2R_1)$, one finds that the generators \mathbf{F}, \mathbf{B} of the group satisfy

$$\begin{aligned} [F_i, F_j] &= +if_{ijk}F_k, \\ [F_i, B_j] &= +if_{ijk}B_k, \\ [B_i, B_j] &= -if_{ijk}F_k. \end{aligned} \quad (8)$$

Consequently our conclusion is that \mathbf{F} indeed generate rotations and \mathbf{B} generate boosts. Moreover, by defining a pair of new non-Hermitian generators $A^\pm \equiv 1/2(\mathbf{F} \pm i\mathbf{B})$ and checking their commutation relations, it can be shown that the hyper-Lorentz group is of the nonchiral SU(3) \times SU(3) type.⁹ In particular, a contravariant vector A^μ transforms according to its (3, 3*) irreducible representation, while a covariant one A_μ transforms via its (3*, 3) irreducible representation.

At this stage, we stress several important points:

(1) The invariant (1) requires $x_\mu \equiv \sqrt{3}g_{\mu\alpha\beta} x^\alpha x^\beta$ to be a covariant vector, and since x^μ and x_μ are linearly independent, there are no g^μ_ν -like tensors possessing the property of raising and lowering indices.

(2) All the structure tensors: δ^μ_ν , $g_{\mu\nu\lambda}$, $g^{\mu\nu\lambda}$, $\epsilon^{\mu\nu\lambda\sigma}$ (for this generalized Levi-Civita tensor, see Appendix A) have the property that $N_u - N_d \equiv 0 \pmod{3}$, where N_u and N_d are the numbers of the up and down indices, respectively.

(3) Any vector can be rotated to the form: $A^\mu = (A^0; 00A^3 0000A^8)$, i.e., we can always choose a preferred plane, namely the (3, 8) plane, but not a preferred single axis as is possible in the ordinary space case.¹⁰ This property follows from the existence of two-diagonal SU(3) generators.

(4) Let $\beta_3 = A$, $\beta_8 = \sqrt{3}B$ be the two boost parameters along the preferred plane direction, then $R = \exp \omega$ is given in its regular form by

$$\begin{aligned} x'^{1,2} &= e^B \cdot x^{1,2}; \quad x'^{4,5} = \exp[(A - B)/2] \cdot x^{4,5}, \\ x'^{6,7} &= \exp[-(A + B)/2] \cdot x^{6,7}, \end{aligned} \quad (9a)$$

showing the 0-3-8 mixing and other properties which are discussed in Sec. VI. This matrix is our internal analog to the famous "external" Lorentz transformation.

Next we define the inhomogeneous hyper-Lorentz, or hyper-Poincaré, transformation by: $x \rightarrow x' = Rx + a$. Nine more translation generators P_μ are introduced, with the following commutation rules:

$$[P_\mu, P_\nu] = 0, \quad (10a)$$

$$[f_{\beta}^{\alpha}, P_\gamma] = -i\epsilon_{\gamma}^{\delta\alpha\beta} P_\delta, \quad (10b)$$

where the tensor f_{β}^{α} of generators is given explicitly in Appendix A. These relations follow from the well-known group property $U(R_2, a_2)U(R_1, a_1) = U(R_2R_1, R_2a_1 + a_2)$.

The principal Casimir operator of the entire group is built in an analogous way to the Lorentzian m^2 , that is

$$M^3 \equiv \sqrt{3}g^{\mu\nu\lambda}P_\mu P_\nu P_\lambda, \quad (11)$$

and for any M^3 ($M^3 > 0$, $M^3 < 0$, $M^3 = 0$) several separated and isolated branches exist, i. e., there is no R to take us from one branch to another. Let us now classify the possible branches, using the preferred plane where $P_\mu = (E; 00p0000q)$.

A. The $M^3 > 0$ (or $M^3 < 0$) case

There exist two distinguishable branches as demonstrated in Fig. 1.

(1) Central branch—it exists only for $E \geq M$ (or for $E \leq M$ for negative M^3) and the intrinsic rest frame $[P_\mu = (M; 0)]$ is contained in it. Any $p_\mu = M(R^{-1})_{\mu}^0$ is a member of this branch.

(2) Peripheral branch—this branch does not contain the rest frame; it exists for any $-\infty < E < +\infty$ and hence has no Lorentzian analog.

B. The $M^3 = 0$ case

Here we shall discuss only the central branch which splits into three separated subbranches, coming from the $M \rightarrow \pm 0$ limit. As it is seen from Fig. 2 the $M = 0$ dispersion surfaces are just the $M^3 \neq 0$ asymptotic planes.

(1) Null frame—where $p_\mu = 0$. This singular point is located at the origin.

(2) Axial subbranch—here $p_\mu \neq 0$, but $p^\mu \equiv \sqrt{3}g^{\mu\nu\lambda}p_\nu p_\lambda = 0$. This subbranch is found to be along the special axes drawn in Fig. 2.

(3) General subbranch—both p_μ and p^μ are different from zero. These subbranch points are at the described regions.

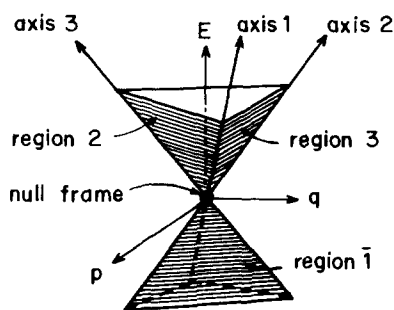


FIG. 2. The $M = 0$ subbranches.

It should be emphasized again that if p belongs to some subbranch, then Rp also belongs to it.

III. THE GROUP INVARIANTS AND THE EXACT SU(3) LIMIT

Let $r(p)$ be a transformation which belongs to the little group of p , i. e., $r(p)p = p$, and let $I + \omega(p)$ be such an infinitesimal transformation. It can be proved that $\omega(p)$ is of the form

$$\omega(p)_{\nu}^{\mu} = \epsilon_{\nu}^{\mu\alpha\beta} \rho_{\alpha} n^{\beta}, \quad (12)$$

for any arbitrary n^{μ} ; so the corresponding unitary operator has the form

$$U(p) = I + iF_{\nu}^{\mu} \epsilon_{\nu}^{\mu\alpha\beta} \rho_{\alpha} n^{\beta} = I + if_{\beta}^{\alpha} \rho_{\alpha} n^{\beta} = I + iW_{\mu} n^{\mu}, \quad (13)$$

where the W_{μ} , the little-group generators, are given explicitly by

$$\begin{aligned} W_0 &= \sqrt{\frac{2}{3}} \mathbf{F} \cdot \mathbf{P}, \\ W_i &= \sqrt{\frac{2}{3}} F_i P_0 + f_{ijk} B_j P_k + d_{ijk} F_j P_k. \end{aligned} \quad (14)$$

These W_{μ} satisfy the familiar (10b) commutation relations:

$$[f_{\beta}^{\alpha}, W_{\gamma}] = -i\epsilon_{\gamma}^{\delta\alpha\beta} W_{\delta}. \quad (15)$$

Now we are able to construct the invariants of the entire group by using the $M^3 \neq 0$ "rest" values:

$$p_{\mu}(\text{rest}) = (M; 0), \quad W_{\mu}(\text{rest}) = \sqrt{\frac{2}{3}} M(0; F). \quad (16)$$

The invariants are

$$\begin{aligned} I_1 &\equiv \sqrt{3}g^{\mu\nu\lambda}P_{\mu}P_{\nu}P_{\lambda} = M^3, \\ I_3 &\equiv -3\sqrt{3}g^{\mu\nu\lambda}W_{\mu}W_{\nu}P_{\lambda} = C_2 M^3, \\ I_4 &\equiv \frac{3}{2}\sqrt{3}g^{\mu\nu\lambda}W_{\mu}W_{\nu}W_{\lambda} = C_3 M^3, \end{aligned} \quad (17)$$

and $I_2 \equiv g^{\mu\nu\lambda}W_{\mu}P_{\nu}P_{\lambda} \equiv 0$ which is an identity. The two coefficients C_2, C_3 are the Casimir operators of SU(3).

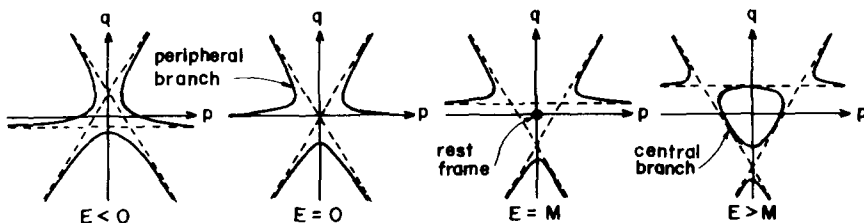


FIG. 1. The $M^3 > 0$ different branches.

From (16) it is clear that the little group associated with the intrinsic rest frame is an SU(3) group, whose representations determine the hyper-Poincaré invariants (17), although we are dealing with a more complicated group. Two quantities are thus needed to label any given state: M^3 —yet without any physical interpretation, and the F spin in the generalized rest frame (16) which we identify as the original SU(3) spin. The internal SU(3) symmetry breaking is obtained by leaving this special frame, through some boost, because the W_μ are no longer pure rotations [there is a boost penetration into its structure, as follows from (14)]. Therefore we assume that *the hyper-Lorentz rest frame is the frame where SU(3) is an exact symmetry*. If mass degeneracy at this limit is the result of a hypothetical switching off of SU(3)-breaking interactions, then any physical hadron must “move” relative to our rest frame, with some principal boost parameters A, B [(9)] along some plane direction chosen to be the preferred one. Such a situation implies, beside an SU(3) breaking, a possible mixing of representations [e. g., the structure of R implies a mixing between the singlet and the octet representations of SU(3)], while the parameters A, B must be somehow related to the coupling constants of the interactions mentioned (a more detailed discussion is brought in Sec. VI).

From what has been said so far one may expect that the $M^3 \neq 0$ central branch contains a possible particle interpretation, but there are several strong arguments against such a possibility:

(1) The nonvanishing of M^3 makes it the dominant quantum number of the theory. Such a quantity can take any continuous value, therefore we cannot think of any candidate for such an intrinsic quantum number.

(2) The rest frame, as a member of the $M^3 \neq 0$ central branch, makes equal-mass multiplets possible. However such multiplets have not been found.

(3) Another difficulty connected with the rest frame is its isotropy, which yields no preferred quantization plane. Such a plane is necessary in order to prevent states, built as linear combinations of different charges, from appearing.

(4) Since M^3 and F complete the states classification, no room is left for a baryon number definition; thus something is still missing in the theory.

These problems can be avoided by the simple assumption that *physical particles have $M=0$* . The rest frame problems disappear because the null frame cannot be reached as explained, and the baryon number appears quite spontaneously and finds its natural place in the scheme, as explained below.

IV. THE BARYON NUMBER AND THE GENERALIZED QUARK MODEL

In the $M=0$ case, the three invariants (17) are not sufficient to characterize the representation [I_3 and I_4 vanish as well as their SU(3) content]. However, in this case, instead of those invariants, a new quantum number can be defined in analogy to the Lorentzian helicity. We identify this quantum number as the bary-

on number, and it is used to label the $M=0$ representations. First we shall study the representations of the proper little group by finding the representations of the Lie algebra of its generators, because the different states furnish these representations. Neglecting the null-frame case, there are two types of finite representations for the two left separated subbranches, respectively.

A. The general subbranch and its related quarks

In the preferred plane p_μ can have one of the three forms which are indicated in Fig. 2:

$$p_\mu = \begin{cases} (- (1/\sqrt{2})q - \sqrt{\frac{3}{2}}p; 00p0000q), & \chi < -1, \\ (- (1/\sqrt{2})q + \sqrt{\frac{3}{2}}p; 00p0000q), & \chi > 1, \\ (\sqrt{2}q & ; 00p0000q), & -1 < \chi < 1, \end{cases} \quad (18)$$

where χ is defined by $\chi \equiv p/\sqrt{3}q$. For demonstration purposes we shall use here the third form, but the same can be done with the two other forms as well. The little-group generators are then given by (see Appendix B):

$$\begin{aligned} J_1 &= (1 - \chi^2)^{-1/2}(F_1 + \chi B_2), & L_4 &= (1 + \chi)^{1/2}(F_4 + B_5), \\ J_2 &= (1 - \chi^2)^{-1/2}(F_2 - \chi B_1), & L_5 &= (1 + \chi)^{1/2}(F_5 - B_4), \\ J_3 &= F_3, & L_6 &= (1 - \chi)^{1/2}(F_6 + B_7), \\ J_8 &= F_8, & L_7 &= (1 - \chi)^{1/2}(F_7 - B_8). \end{aligned} \quad (19)$$

By examining the commutation relations one finds the existence of four translations (L) which form an invariant Abelian subalgebra, and four rotations (J) out of which two are diagonal, so the total algebra generated is not semisimple. In order that the states will form a finite set, it is necessary to represent the translations by zero, and to allow only SU(3) singlets. Taking these requirements into account (Appendix C), it then follows from the explicit form (B2) of the W_μ that the two vectors P_μ and W_μ are proportional,

$$W_\mu = -\lambda P_\mu. \quad (20)$$

The proportion coefficient λ is the new invariant mentioned before, and it is given explicitly by

$$\lambda = -\frac{W_0}{P_0} = -\sqrt{\frac{2}{3}} \frac{pF_3 + qF_8}{p_0(p, q)}, \quad (21)$$

where the various $p_0(p, q)$ are given by (18). A deeper inspection (Appendix C) shows that for any given λ we can use only the $[(a, 0); (0, b)]$, $[(0, b); (a, 0)]$ hyper-Lorentz representations when p_μ, p^μ are at the general sub-branch respectively. For both

$$\lambda = \frac{1}{3} \cdot (a - b), \quad (22)$$

which is the generalized Weinberg theorem.¹¹ By considering the simplest representations ($a=0$ or $b=0$) we can summarize:

- (1) λ uniquely determines the SU(3) representation.
- (2) Only triangular representations are allowed.
- (3) The possible populated states are located only at the representation vertices.
- (4) Any allowed state is related to only one form of p_μ [the invariant λ must be independent of χ in (21)].

These limitations⁹ prevent the *direct* population of the physical known SU(3) multiplets. The 3 and 3* representations are the only permitted representations that are possibly fully populated; thus the quark model provides the only consistent picture. The quarks (anti-quarks) are then described as members of the 3(3*) representation of SU(3), belonging to the $M=0$ general subbranch. Furthermore, note that

$$\lambda(3) = +\frac{1}{3}; \lambda(3^*) = -\frac{1}{3}, \quad (23)$$

so there is almost no other possibility but to get the desired connection

$$B \equiv \lambda, \quad (24)$$

which highly suggests that the baryon number B is essentially a component of the F spin along the hyper momentum direction.

B. The axial subbranch and its pseudoquarks

In our opinion, this case can contain a possible origin of the hadronic weak interaction because of the strange algebra generated by the little-group generators. To begin with, we write the three possible p_μ in the preferred plane, following Fig. 2. They involve only a single parameter (and not two, as in the previous case)

$$p_\mu = \begin{cases} (\sqrt{2}q; 00\sqrt{3}q0000q), & \chi = +1 \\ (\sqrt{2}q; 00-\sqrt{3}q0000q), & \chi = -1 \\ (-\frac{1}{\sqrt{2}}q; 0000000q), & \chi = 0. \end{cases} \quad (25)$$

The little-group effective¹² generators are *only five now, and not eight!* (it follows from the structure of the W_μ shown in Appendix B). They include four translations and only one rotation which is also diagonal. For example, using the first form of p_μ , the generators are

$$\begin{aligned} L_1 &= F_1 + B_2, & L_2 &= F_2 - B_1, & L_4 &= F_4 + B_5, \\ L_5 &= F_5 - B_4, & Q &= F_3 + (1/\sqrt{3})F_8. \end{aligned} \quad (26)$$

By making use of previous arguments we can show that (20) and (24) still hold, while the representations are different now. A given λ is connected only with those $[(a_1, b_1); (a_2, b_2)]$ representations satisfying the relations $\frac{1}{3}(a_1 + 2b_1) - \frac{1}{3}(2a_2 + b_2) = \lambda$ or $-\frac{1}{3}(2a_1 + b_1) + \frac{1}{3}(a_2 + 2b_2) = \lambda$ depending on whether p_μ or p^μ are at the axial subbranch, respectively (see Appendix C). For the simplest representations ($a_1, b_1 = 0$ or $a_2, b_2 = 0$) we obtain the following properties:

(1) Except for the trivial cases $\lambda = 0, \pm \frac{1}{3}$, λ does not determine the SU(3) representations in a unique way [e. g., (1;1) and (0;3) are both $\lambda = 1$ cases]!

(2) The possible occupied states are located at the representation periphery.

(3) These states are SU(2) degenerated, a property which results from the three vanishing rotation generators.

Consider, for example, the three possible states for $\lambda = \frac{1}{3}$ (or $B = \frac{1}{3}$):

$$\begin{aligned} &|\cos\theta_1 \cdot d + \sin\theta_1 \cdot s\rangle \text{ for } \lambda = -F_3 - \frac{1}{2}Y = \frac{1}{3}, \\ &|\cos\theta_2 \cdot s + \sin\theta_2 \cdot u\rangle \text{ for } \lambda = F_3 - \frac{1}{2}Y = \frac{1}{3}, \\ &|\cos\theta_3 \cdot u + \sin\theta_3 \cdot d\rangle \text{ for } \lambda = +Y = \frac{1}{3}, \end{aligned} \quad (27)$$

where the angles θ are yet undetermined and can take any continuous value. Among these three possibilities only the first one seems to have particle interpretation, because the two others have no defined Q , while in nature all known particles have definite charges. Let us list some of the so-called pseudoquark [the first state in (27)] properties:

(1) Only one diagonal SU(3) generator (namely Q) characterizes it; therefore it transforms like a one-dimensional representation.

(2) The pseudoquark state is a d - s mixture.

(3) There exist two different pseudoquarks: one, which is described by p_μ and has $g^{\mu\nu\lambda}p_\nu p_\lambda = 0$, and the other described by p^μ and satisfies $g_{\mu\nu\lambda}p^\nu p^\lambda = 0$.

These properties are clearly leptonic ones; so we might expect the pseudoquarks to be associated with weak interactions. One can even speculate that these objects have something to do with the structure of the leptons. The possible existence of a single pseudoquark out of three allowed ones reminds us of the neutrino on the SU(2) level. This $m^2 = 0$ particle occurs in only one helicity state; thus the hyper-Lorentz pseudoquark is our analog of the neutrino.

V. A NAIVE MODEL OF QUARK INTERACTIONS

The model proposed here is a qualitative one, although it has some important basic properties. The strong interaction of quarks is described by an "effective Lagrangian" which is a hyper-Lorentz scalar. This scalar is built from quark currents, in analogy to the well known effective Lagrangian of the weak interaction, but yet no space-time meaning is given to the quantities involved.

The model is based on two mathematical properties that were first presented in Sec. II:

(1) The raising and lowering indices operations are absent.

(2) The metric tensor is a third order one, with its indices either all up or all down.

The first property implies two different currents: J_μ and J^μ . These currents are written as

$$J^\mu = \bar{\psi}(F^\mu + \dots)\psi, \quad J_\mu = \bar{\phi}(F_\mu + \dots)\phi, \quad (28)$$

where the creation and annihilation operators are related to quark (ψ) and antiquark (ϕ) fields, and where $F^\mu = [(1/\sqrt{6})I; \mathbf{F}^3]$ $F_\mu = [-(1/\sqrt{6})I; \mathbf{F}^{3*}]$. The second property allows us to form interactions of different types that contain N contravariant currents and \bar{N} covariant ones, such that $N - \bar{N} = 0 \pmod{3}$. In the lowest order, three basic interactions are possible; only one of which reminds us of the Fermi interaction:

$$f_M \cdot J_\mu J^\mu, \quad f_B \cdot g_{\mu\nu\lambda} J^\mu J^\nu J^\lambda, \quad f_{\bar{B}} \cdot g^{\mu\nu\lambda} J_\mu J_\nu J_\lambda, \quad (29)$$

where $f_M, f_B, f_{\bar{B}}$ are coupling constants. They corre-

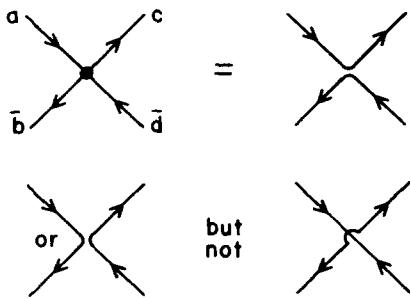


FIG. 3. Diagrams for the quark reaction $a + \bar{b} \rightarrow c + \bar{d}$.

spond, respectively, to situations where a quark-anti-quark pair, three quarks and three antiquarks entering and coming out of the interaction vertex.

The main points of this model are the following ones:

(1) The current structure and the F-spin conservation at the interaction vertex make it possible to graphically describe the interaction by continuous quark lines that enter duality diagrams. The simplest example, drawn in Fig. 3, describes the quarks reaction $a + \bar{b} \rightarrow c + \bar{d}$, which is of the $J_\mu J^\mu$ type. The SU(3) quantum numbers of a and c (and therefore b and d) or of a, b (and c, d) must be the same, although they may differ in their hypermomentum p . The third possibility $a = d, b = c$ is forbidden because a quark creation and an antiquark annihilation do not form a current (3×3 does not contain 1, 8). This property may turn out to be connected to the drawing rules of duality diagrams.

(2) n quarks and \bar{n} antiquarks can interact together only if $n - \bar{n} \equiv 0 \pmod{3}$. If we assume that any real particle is just a bound state of these interacting quarks, then this model is a mathematical mechanism which explains the low-lying triality zero ($l=0$) states and prevent other $l \neq 0$ quark combinations from appearing. Still exotic states do exist (e.g., via the $g_{\mu\nu\alpha\beta} g^{\alpha\lambda\gamma} J_\mu J_\lambda J^\nu J_\gamma$ interaction, etc.); thus one must postulate that the interaction among quarks is done *only* according to the three simple possibilities (29) if he wants to get rid of those unpopular states. This assumption is consistent with the fact that only $B=0, \pm 1$ elementary particles appear in nature.

(3) The existence of bound states can be explained by assuming large coupling constants ($f_M, f_B, f_{\bar{B}}$). In such a way, high-order processes will dominate the low-order ones, and quarks leaving some vertex must interact again and again infinite numbers of times. This idea is illustrated in Fig. 4, where we made use of the Zweig rule (a), which can be formulated here as follows: *a quark line does not interact with itself* [the violation of the rule is shown in (b)]. Perhaps this rule is hidden somewhere in the model (it may be connected with current contractions) but unfortunately we have not been able to find it.

(4) Our naive model says nothing about the existence or nonexistence of free quarks, but it can be easily generalized to contain the concept of gluons. It is possible to introduce them into the model by giving up the locality of the interaction in the nine-dimensional

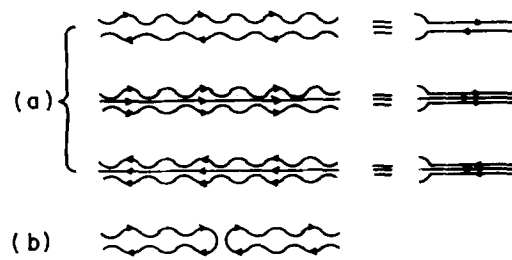


FIG. 4. (a) The fundamental bound states. (b) The Zweig rule violation.

space. $J^\mu J_\mu \rightarrow J^\nu G_{\nu\lambda}^\mu J_\mu$ and $g_{\mu\nu\lambda} J^\mu J^\nu J^\lambda \rightarrow G_{\mu\nu\lambda} J^\mu J^\nu J^\lambda$, where G are some "gluon internal propagators" reminding us of the weak interaction W boson propagator.

VI. THE MASS OPERATOR AND THE PROPOSED SYMMETRY

From the Lorentzian point of view, the mass operator is a *quadratic* scalar independent of the particle spin. On the other hand, any typical hyper-Lorentz scalar [e.g., (17)] has a *cubic* structure (unlike the quadratic scalars of SU(3)). This difference in dimensions between scalars of the two families is, in our opinion, the reason why the mass operator cannot be an invariant under both the Lorentz and the hyper-Lorentz transformations. We therefore assume that the mass operator is a Lorentz scalar whose values are determined by intrinsic hyper-Lorentz properties. Below we discuss qualitatively such possible operators.

In the exact symmetry limit one expects mass degeneracy within a given SU(3) multiplet; in our language it is to say that *the mass operator is a rotational invariant only in the intrinsic rest frame*. The boost transformation which takes us out of this frame is shown explicitly in (9). It consists of two parameters A, B which represent an internal motion along the 3, 8 directions, respectively. Nonets (but not octets and singlets separately) are naturally related to this 9×9 transformation. One can easily notice three basic properties of (9) which are able to connect it with masses of a nonet members.

(1) The transformation obeys the so-called R symmetry, i.e., polar nonet states are multiplied by the same coefficients.

(2) The choice $A=0$ implies the appearance of an exact $SU(3)_T$ symmetry.

(3) There is a 0-3-8 mixing, which converges to a 0-8 one in the $A=0$ limit. Besides showing a possible origin to mass formulas for nonets, these properties suggest the *identification of A as an electromagnetic parameter and of B as a medium-strong one*.

The mass operator must be kept as a rotational invariant as long as we stay in the intrinsic rest frame. This property suggests to construct it as some zero component of a hyper-Lorentz tensor of operators. In such a way it will be proportional to the identity only in the exact symmetry limit, but any given boost will contribute some SU(3) symmetry-breaking terms.

Consider, for example, a $m+n$ order tensor $M_{\nu_1 \dots \nu_n}^{\mu_1 \dots \mu_m}$ whose $\mu, \nu=0$ component is assumed to be the "bare" mass operator (and therefore proportional to I). By applying a hyper-Lorentz transformation to this quantity, we obtain the "renormalized" mass operator \hat{m}^2 ,

$$\hat{m}^2 = M_{0 \dots 0}^{0 \dots 0} = R_{\mu_1}^0 \dots R_{\mu_m}^0 (R^{-1})_{\nu_1}^0 \dots (R^{-1})_{\nu_n}^0 \quad (30)$$

$$\times M_{\nu_1 \dots \nu_n}^{\mu_1 \dots \mu_m}$$

expressed by the original M terms. There is no need for the proposed mass operator (30) to be a universal operator. The number of its indices and their location can as well express the quark content of the particles considered. For example,

$$\begin{aligned} \hat{m}^2 (\text{mesons}) &\equiv M_{0'}^{0'}, \\ \hat{m}^2 (\text{baryons}) &\equiv M^{000'}, \\ \hat{m}^2 (\text{antibaryons}) &\equiv M'_{000}. \end{aligned} \quad (31)$$

Since we can choose the boost to be along the preferred plane (3, 8 plane) direction, R takes the form (9) and the μ, ν indices in (30) are only 0, 3, 8. Physically it means that m^2 receives pure and mixed electromagnetic and medium-strong contributions.

Finally we remark that the concept of charm does not appear in this paper because our proposed symmetry is based on SU(3). However, a similar generalization can be applied to SU(4). This idea will be considered in a future paper.

ACKNOWLEDGMENTS

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APPENDIX A: THE GENERALIZED LEVI-CIVITA TENSOR

The generalized Levi-Civita tensor is given explicitly by

$$\epsilon \text{ (one or more indices are 0)} = 0, \quad (A1)$$

$$\epsilon_{i^* j^* k^*}^{0^* j^* k^*} = \epsilon_{i^* j^* k^*}^{i^* j^* k^*} = \epsilon_{i^* j^* k^*}^{i^* j^* k^*} = \sqrt{\frac{2}{3}} f_{ijk}$$

$$\epsilon_{j^* k^* l^*}^{i^* k^* l^*} = f_{ijk} d_{phl} + d_{ijp} f_{phl},$$

and it has the following properties:

$$g^{\alpha\nu\sigma} \epsilon_{\nu\sigma}^{\mu\lambda} = g_{\alpha\mu\lambda} \epsilon^{\mu\lambda}_{\nu\sigma} = 0, \quad (A2)$$

$$\epsilon_{\alpha^* \gamma^*}^{\mu^* \beta^*} \cdot \epsilon_{\beta^* \nu^*}^{\alpha^* \gamma^*} = 16 \delta_{\nu}^{\mu},$$

$$\epsilon_{\alpha^* \beta^*}^{\mu^* \beta^*} = -\epsilon_{\alpha^* \beta^*}^{\nu^* \mu^*} = -\epsilon_{\beta^* \alpha^*}^{\mu^* \nu^*},$$

$$(\epsilon_{\nu^* \sigma^*}^{\mu^* \lambda^*})' = \epsilon_{\nu^* \sigma^*}^{\mu^* \lambda^*},$$

We use this tensor in order to build the tensor f_{α}^{μ} = $\epsilon_{\nu^* \beta^*}^{\mu^* \beta^*} F_{\alpha}^{\nu}$ of generators (10b), and one finds

$$\begin{aligned} f_{0}^0 &= 0, \\ f_{i^*}^0 &= f_{i^*}^0 = \sqrt{\frac{2}{3}} F_i, \\ f_{j^*}^i &= f_{ijk} B_k + d_{ijk} F_k. \end{aligned} \quad (A3)$$

APPENDIX B: THE LITTLE-GROUP GENERATORS

In the preferred plane, where $p_{\mu} = (E; 00p0000q)$, W_{μ} are given explicitly by

$$\begin{aligned} W_0 &= \sqrt{\frac{2}{3}} (pF_3 + qF_8), \\ W_{1,2} &= [\sqrt{\frac{2}{3}} E + (1/\sqrt{3})q] F_{1,2} \pm pB_{2,1}, \\ W_3 &= [\sqrt{\frac{2}{3}} E + (1/\sqrt{3})q] F_3 + (1/\sqrt{3})pF_8, \\ W_{4,5} &= [\sqrt{\frac{2}{3}} E + \frac{1}{2}p - (1/2\sqrt{3})q] F_{4,5} \pm (\frac{1}{2}p + (\sqrt{3}/2)q) B_{5,4}, \\ W_{6,7} &= [\sqrt{\frac{2}{3}} E - \frac{1}{2}p - (1/2\sqrt{3})q] F_{6,7} \pm [-\frac{1}{2}p + (\sqrt{3}/2)q] B_{7,6}, \\ W_8 &= [\sqrt{\frac{2}{3}} E - (1/\sqrt{3})q] F_8 + (1/\sqrt{3})pF_3. \end{aligned} \quad (B1)$$

At the $M=0$ general subbranch, where $p_{\mu} = (\sqrt{2}q; 00p0000q)$, W_{μ} become somewhat simpler

$$\begin{aligned} W_0 &= \sqrt{\frac{2}{3}} (pF_3 + qF_8) = \sqrt{2} W_3, \\ W_{1,2} &= \sqrt{3} q F_{1,2} \pm p B_{2,1}, \\ W_3 &= \sqrt{3} q F_3 + (1/\sqrt{3}) p F_8, \\ W_{4,5} &= [(\sqrt{3}/2)q - \frac{1}{2}p] (F_{4,5} \pm B_{5,4}), \\ W_{6,7} &= [(\sqrt{3}/2)q - \frac{1}{2}p] (F_{6,7} \pm B_{7,6}), \end{aligned} \quad (B2)$$

and the simplest form of W_{μ} is obtained at the $M=0$ axial subbranch where $p_{\mu} = q(\sqrt{2}; 00\sqrt{3}00001)$:

$$\begin{aligned} W_0 &= \sqrt{2} q Q = \sqrt{\frac{2}{3}} W_3 = \sqrt{2} W_8, \\ W_{1,2} &= \sqrt{3} q (F_{1,2} \pm B_{2,1}), \\ W_{4,5} &= \sqrt{3} q (F_{4,5} \pm B_{5,4}), \\ W_{6,7} &\equiv 0. \end{aligned} \quad (B3)$$

APPENDIX C: THE GENERALIZED WEINBERG THEOREMS

Using the operators $A^{\pm} = \frac{1}{2}(F \pm iB)$ we have shown in Sec. II that the hyper-Lorentz group is of the nonchiral SU(3) \times SU(3) type. Let us now express the little-group generators in terms of those non-Hermitian generators A^{\pm} , first at the general subbranch (19), and then at the axial one (26). By using

$$F = A^+ + A^-, \quad B = -i(A^+ - A^-)$$

one gets at the general subbranch:

$$\begin{aligned} J_{1,2} &= (1 - \chi^2)^{-1/2} [(A_{1,2}^+ \mp i\chi A_{2,1}^+) + (A_{1,2}^- \pm i\chi A_{2,1}^-)], \\ J_{3,8} &= A_{3,8}^+ + A_{3,8}^-, \\ L_{4,5} &= (1 + \chi)^{1/2} [(A_{4,5}^+ \mp iA_{5,4}^+) + (A_{4,5}^- \pm iA_{5,4}^-)], \\ L_{6,7} &= (1 - \chi)^{1/2} [A_{6,7}^+ \mp iA_{7,6}^+] + (A_{6,7}^- \pm iA_{7,6}^-). \end{aligned} \quad (C1)$$

Next we define T^{\pm} , V^{\pm} , U^{\pm} as the SU(2) generators of A^{\pm} . The limitations which follow from the requirement of having a finite set of states, mentioned in Sec. IV, are

$$T_3^+, V_3^+, U_3^+ |\lambda\rangle = 0, \quad (\text{C2})$$

$$T_3^-, V_3^-, U_3^- |\lambda\rangle = 0, \quad (\text{C3})$$

$$(T_3^+ + T_3^-) |\lambda\rangle = 0, \quad (\text{C4})$$

$$(Y^+ + Y^-) |\lambda\rangle = -2\lambda |\lambda\rangle. \quad (\text{C5})$$

Therefore, if we consider an $[(a_1, b_1); (a_2, b_2)]$ hyper-Lorentz representation, then

$$(C2) \Rightarrow b_1 = 0, \quad (C3) \Rightarrow a_2 = 0, \quad (C5) \Rightarrow \frac{1}{3}a_1 - \frac{1}{3}b_1 = \lambda. \quad (\text{C6})$$

These relations are just the generalized Weinberg theorem and the general subbranch properties discussed in Sec. IV.

At the axial subbranch the situation is simplified, and after some substitutions similar to (C1) one gets the following restrictions:

$$T_3^+, V_3^+ |\lambda\rangle = 0, \quad (\text{C7})$$

$$T_3^-, V_3^- |\lambda\rangle = 0, \quad (\text{C8})$$

$$(Q^+ + Q^-) |\lambda\rangle = -\lambda |\lambda\rangle. \quad (\text{C9})$$

(C9) is again the proper Weinberg theorem, and (C7), (C8) give some other representation properties; but the more important point here is the $SU(2)_U$ degeneracy

following from the survival of only five little-group generators in this case.

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⁸As proposed by M. Gell-Mann and M. Levy, Nuovo Cimento **16**, 705 (1960).

⁹For the "external" analog see, for example, S. Weinberg, Phys. Rev. **133**, 1318 (1964).

¹⁰Where we are always able to choose any preferred axis as our \hat{z} axis.

¹¹S. Weinberg, Phys. Rev. **134**, 882 (1964). This theorem proves that for $m^2=0$ and a given helicity λ only the $(A; B)$ representations of the Lorentz group, with $\lambda = -A + B$, are available.

¹²There exist 11 degrees of freedom in this case, only five of which are connected with the W_μ . The other six generators are irrelevant since they act on definite zeroes of the p_μ .

Relativistic spherical stars reformulated

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The problem of finding static, spherically symmetric, solutions of Einstein's equations for a perfect fluid is reformulated. A field equation connecting the pressure and density and free of metric components is obtained. Upon finding a solution of this field equation, the metric components are then obtained by quadrature. A solution-generating technique is developed which yields physically valid pressure-density configurations for adiabatically stable stars. Analytic solutions are obtained for the pressure, density, and metric components.

1. INTRODUCTION

There are two traditional approaches to finding the configurations of static spherical stars. The Oppenheimer-Volkoff method¹ consists of simultaneous numerical integration of the Einstein field equations for pressure and mass. An explicit equation of state is assumed, and the integration starts at the center of the star with a prescribed central pressure. The integrations are iterated until the pressure decreases to zero, indicating the surface of the star has been reached.

Analytic configurations can be obtained by Tolman's method,² wherein one of the two metric components is chosen as some explicit function of the radial coordinate and one of the Einstein field equations is then integrated to find the other metric component. Both components are then substituted into the remaining field equations to obtain the pressure and density. As might be expected with Tolman's method, unphysical pressure-density configurations are found more frequently than physical ones. Other efforts³⁻⁵ at solution generating are similar to Tolman's approach.

In this work we take the viewpoint that the interior Schwarzschild geometry is of secondary interest, and that pressure and density are the primary quantities. If a physically valid pressure-density configuration can be found, then one is interested in knowing the metric. While the Oppenheimer-Volkoff method is perfectly adequate for obtaining numerical models, there remains some additional understanding to be gained from exact analytic solutions. To this end, the problem has been reformulated⁶ so that one can first find a valid physical configuration and then obtain the metric.

The paper is organized as follows: In Sec. 2 the metric and field equations are given in isotropic coordinates. New metric components are defined in Sec. 3, which cast one of the field equations into a form symmetric in the new metric components. The question of how the physical configurations differ under interchange of the metric components motivates the definitions of the next section. In Sec. 4, two dimensionless quantities, e and f , are defined solely in terms of the pressure and density. From the field equations, a differential equation relating e and f , and free of metric components, is obtained. It is then shown that the met-

ric components can be obtained by quadrature from e and f . In Sec. 5 the Newtonian limit of the e - f equation is obtained and shown to agree with the appropriate Newtonian equation for spherical equilibrium. Since the e - f equation is nonlinear and difficult to solve, a solution-generating technique is formulated in Sec. 6. Conditions are given for physically valid pressure-density configurations, and an algorithm is then given for generating physically valid solutions. An example is given, and a formula is presented for the total mass.

2. FIELD EQUATIONS

We consider a static spherically symmetric space-time with a perfect fluid source. The metric is written in isotropic coordinates:

$$ds^2 = A^2 dt^2 - B^2 [d\rho^2 + \rho^2 (d\theta^2 + \sin^2\theta d\varphi^2)], \quad (1)$$

where $A = A(\rho)$, $B = B(\rho)$. The Einstein equations for a perfect fluid are

$$R_{\mu\nu} - \frac{1}{2}g_{\mu\nu}R = -8\pi[(\mu + p)u_\mu u_\nu - pg_{\mu\nu}], \quad (2)$$

where $u^\mu = A^{-1}\delta_t^\mu$ is the unit tangent to the matter flow and lies along the timelike Killing vector δ_t^μ . Isotropy of the pressure and the field equations yield

$$A''/A + B''/B = (A'/A + B'/B)(\rho^{-1} + 2B'/B), \quad (3)$$

where primes denote derivatives with respect to ρ . The pressure p and mass-energy density μ are given by

$$8\pi p = B^{-2} [2(A'/A + B'/B)(\rho^{-1} + B'/B) - (B'/B)^2], \quad (4)$$

$$8\pi\mu = B^{-2} [(B'/B)^2 - 4\rho^{-1}(B'/B) - 2(B''/B)]. \quad (5)$$

The equations of motion yield the Euler equation

$$p' / (\mu + p) = -A'/A. \quad (6)$$

Equation (6) is determined by the field equations (3), (4), and (5), and cannot be counted as a separate field equation.

The system of equations (3), (4), and (5) is completed by choosing any one of the unknowns A , B , p , or μ as a function of ρ or by specifying an equation of state $p = p(\mu)$.

3. SYMMETRIC FIELD VARIABLES

To find an equation relating p and μ without metric variables we proceed by stages, first introducing new

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metric components:

$$E/D := A, \quad D^2 := B. \quad (7)$$

The field equations are rewritten as

$$D''/D + E''/E - 6(D'/D)(E'/E) - \rho^{-1}(D'/D + E'/E) = 0, \quad (8)$$

$$8\pi p = 2D^{-4}[2(D'/D)(E'/E) + \rho^{-1}(D'/D + E'/E)], \quad (9)$$

$$8\pi\mu = -4D^{-5}(D'' + 2\rho^{-1}D'), \quad (10)$$

$$p' / (\mu + p) = D'/D - E'/E. \quad (11)$$

Note that field equation (8) is invariant under

$$\rho \rightarrow (\alpha\rho^2 + \beta)^{1/2}$$

for constants α and β . Equation (8) is also bilinear in D and E and invariant under $E \rightarrow D$, $D \rightarrow E$. Since p and μ change under $D \rightleftharpoons E$, we are led to the question of whether both solutions (E, D) and (D, E) can correspond to valid physical configurations and hence are led to the new variables in the following section.

4. PRESSURE AND DENSITY AS PRIMARY VARIABLES

It is convenient to define two dimensionless variables which depend only on the pressure and density:

$$e := \rho p' / (\mu + p), \quad (12)$$

$$f := p / (\mu + 3p).$$

From Eq. (11), it follows that

$$e = \rho(D'/D - E'/E). \quad (13)$$

Equations (8), (9), and (10) yield

$$f' = \frac{2(D'/D)(E'/E) + \rho^{-1}(D'/D + E'/E)}{E''/E - D''/D - 2\rho^{-1}(D'/D - E'/E)}. \quad (14)$$

The new variables e and f should be negative and positive, respectively, for a valid physical configuration (see Sec. 6). Under $D \rightleftharpoons E$, it follows from (13) and (14) that $e \rightarrow -e$, $f \rightarrow -f$. Thus, if a (D, E) solution corresponds to a valid physical configuration, then the solution $D \rightleftharpoons E$ must correspond to an unphysical one.

It is now possible to obtain a single differential equation relating e and f and free of metric variables. Introducing the dimensionless variable u ,

$$u := \rho(D'/D + E'/E), \quad (15)$$

and using (13), the field equation (8) becomes

$$\rho u' - 2u - u^2 + 2e^2 = 0. \quad (16)$$

The physical variable f is now given by

$$f = (e^2 - 2u - u^2) / 2(e + eu + \rho e'). \quad (17)$$

Solving Eq. (17) for u yields

$$u = -(1 + ef) + [1 + e^2(1 + f^2) - 2\rho fe']^{1/2}, \quad (18)$$

where it will be shown (in the Newtonian limit) that the positive square root is required. Substituting Eq. (18) into field equation (16) yields the desired pressure-

density relation:

$$\begin{aligned} & [1 + e^2(1 + f^2) - 2\rho fe']^{1/2} (\rho e f' - \rho e' f + 2e^2 f^2 - e^2) \\ & = \rho e^2 f f' - \rho e' (\rho f' + e f^2 + f - e) - \rho^2 e'' f \\ & \quad + 2ef + 2e^3 f(1 + f^2). \end{aligned} \quad (19)$$

Once a solution of Eq. (19) is found the metric is obtained by quadrature⁷:

$$A'/A = -\rho^{-1}e, \quad (20)$$

$$B'/B = \rho^{-2} \{ e(1-f) - 1 + [1 + e^2(1 + f^2) - 2\rho fe']^{1/2} \}, \quad (21)$$

which follows from Eqs. (6), (13), (15), (18) and definition (7). The pressure and density are recovered from definition (12):

$$\begin{aligned} p &= \exp \left[\int \rho^{-1} e (f^{-1} - 2) dp \right], \\ \mu &= p (f^{-1} - 3). \end{aligned} \quad (22)$$

A straightforward physical approach to spherical stars can now consist of specifying an equation of state $p = p(\mu)$, and then, by solving Eq. (19), a third order nonlinear differential equation, for $\mu(\rho)$. The metric is then determined from Eqs. (20) and (21).

5. THE NEWTONIAN LIMIT

With the speed of light appearing explicitly,

$$e = \rho p' / (\mu c^2 + p),$$

$$f = p / (\mu c^2 + 3p).$$

Dividing by f^2 , Eq. (19) can be rewritten as

$$\begin{aligned} & [1 + e^2(1 + f^2) - 2\rho fe']^{1/2} [2e^2 - (e/f)^2 - \rho(e/f)'] \\ & = 2(e/f) [1 + e^2(1 + f^2)] - \rho^2 f^{-2} (fe')' - \rho ef(e/f)' \\ & \quad + \rho(e'/f)(e/f - 1). \end{aligned}$$

In the limit $c \rightarrow \infty$, one obtains

$$\begin{aligned} & \rho^3 [- (p'''/p) + 3(p''/p)(\mu'/\mu) - 3(p'/p)(\mu''/\mu)^2 \\ & \quad + (p'/p)(\mu''/\mu)] + \rho^2 [4(p'/p)(\mu'/\mu) \\ & \quad + (2/\rho)(p'/p) - 2(p''/p)] = 0. \end{aligned} \quad (23)$$

The Newtonian equations for spherical equilibrium are

$$\frac{dm}{dr} = 4\pi\mu r^2, \quad (24)$$

$$\frac{dp}{dr} = -\frac{Gm}{r^2} \mu.$$

Eliminating the mass yields

$$\mu^{-2} [-p'' + p'(\mu'/\mu) - 2p'/r] = 4\pi G.$$

Differentiating once more and then multiplying by $r^3 \mu^2/p$ provides the Newtonian equation with which Eq. (23) agrees ($\rho \rightarrow r$ in the Newtonian limit). The Newtonian limit shows that the positive square root was required in Eq. (18).

6. SOLUTION GENERATING

Since Eq. (19) is manifestly difficult to solve, we develop a solution-generating technique which yields physically valid pressure-density configurations. Let $u(\rho)$ in Eq. (16) be chosen as a solution-generating func-

tion; then

$$\begin{aligned} 2e^2 &= 2u + u^2 - \rho u', \\ f &= (e^2 - 2u - u^2)/2(e + eu + \rho e'). \end{aligned} \quad (25)$$

The boundary of the star ρ_b is given by $p(\rho_b) = 0$, and the following conditions must hold for a physically valid configuration⁸:

- (i) μ and p must be finite and positive for $0 \leq \rho < \rho_b$;
- (ii) μ and p must decrease outward;
- (iii) $p < \mu$ for $0 \leq \rho < \rho_b$;
- (iv) $0 < dp/d\mu < 1$ for $0 \leq \rho < \rho_b$.

The physical constraints imply that

$$e \leq 0, \quad 0 \leq f < \frac{1}{4}, \quad (26)$$

since e must be negative for p to decrease outward and $p < \mu$ implies that $f < \frac{1}{4}$ directly from the definition of f , and in addition f must be positive. The condition that the speed of sound be less than the speed of light implies, using definition (12),

$$\rho f' > e(1 - 2f)(1 - 4f). \quad (27)$$

The functional form of u is severely restricted by the condition that p and μ be finite at the origin. From Eq. (25), f can be rewritten as

$$f = -e(3u^2 + 2u + \rho u') / (2u^3 + 6u^2 + 4u - \rho^2 u'' - \rho u').$$

The pressure is given by

$$8\pi p = \rho^{-2} D^{-4} (\rho u' + e^2) = \rho^{-2} D^{-4} (u^2 + 2u - e^2)$$

upon substituting Eqs. (13), (15), and (16) into (9). Assuming D to be finite and nonzero at the origin, it then follows that the only functional forms for u and e consistent with p and f finite and nonzero at $\rho = 0$ are

$$u = 0(\rho^2), \quad e = 0(\rho^2) \quad \text{as } \rho \rightarrow 0.$$

Furthermore, since $u(u+2) \geq 0$ follows from the pressure equation, $u = 0(\rho^2)$ as $\rho \rightarrow 0$ implies that $u \geq 0$.

Equation (25) shows that $e^2 = O(\rho^4)$ as $\rho \rightarrow 0$ if and only if u is chosen such that $u = O[\rho^2(\alpha\rho^k + \beta)]$ as $\rho \rightarrow 0$ for constants α, β , and $k \geq 2$ (when $k=2$, α and β must be chosen such that $\beta^2 - 2\alpha \neq 0$). Choosing u positive with a finite first maximum to the right of $\rho = 0$ guarantees that $\rho^{-2}(\rho u' + e^2)$ (and hence the pressure) is positive and finite for $0 \leq \rho < \rho_b$ since ρ_b is given by $\rho u' + e^2 = 0$.

In order to satisfy constraints (26) and (27) at $\rho = 0$, u must have the form $u = O[\rho^2(q - \frac{1}{2}aq^2\rho^2 + \frac{1}{4}bq^3\rho^4)]$ as $\rho \rightarrow 0$ for nonzero constants a, b , and q .

$$a > 23/9 \quad (28a)$$

guarantees $0 < f(0) < \frac{1}{4}$, and if a and b satisfy

$$25b^2 + 10b(12 + 17a) - (18 + 78a + 197a^2 + 162a^3) > 0, \quad (28b)$$

then $0 < dp/d\mu < 1$ at $\rho = 0$.

The following algorithm generates physically valid configurations:

(a) Choose u such that $u = O[\rho^2(q - \frac{1}{2}aq^2\rho^2 + \frac{1}{4}bq^3\rho^4)]$ as $\rho \rightarrow 0$ and $u \geq 0$, with a finite first maximum to the

right of $\rho = 0$, and with a and b satisfying constraint (28);

(b) calculate e^2 from Eq. (25);

(c) find ρ_b from the equation $\rho u' + e^2 = 0$. Demanding ρ_b positive may fix some parameter in u ;

(d) choose $e = -(e^2)^{1/2}$;

(e) calculate f from Eq. (25).

(f) obtain p, μ and the metric components from Eqs. (20), (21), and (22).

Example: The scale freedom of Eq. (25) is used to define the variable $x := \rho/\alpha$ with $\alpha > 0$. Choose $u = 2x^2(1-x^2)/F$ where $F(x) := \beta^2(2+\delta) - (\beta^2\delta+1)x^2 + x^4$, with β, δ constant. Constraint (28) requires

$$\beta^2 > 16/9,$$

$$(5\beta^2\delta - 7)^2 > (18\beta)^2.$$

$$e = -2\beta x^2/F.$$

$$x_b^2 = 1 + \frac{3}{2}\delta^{-1}[1 - (1 + \frac{4}{3}\delta)^{1/2}], \quad \text{requiring } \delta > -\frac{3}{4}.$$

$$f = \frac{\beta[2 + \delta - (3 + 2\delta)x^2 + \delta x^4]}{3\beta^2(2 + \delta) + (1 - \beta^2\delta)x^2 - 3x^4}.$$

$$p/p_0 = \beta^2[2 + \delta - (3 + 2\delta)x^2 + \delta x^4]F^{-1}(H/H_0)^{\beta^2\delta + 2\beta - 1}/\gamma,$$

$$\mu/\mu_0 = [\beta/3(\beta - 1)]JF^{-1}(H/H_0)^{\beta^2\delta + 2\beta - 1}/\gamma,$$

where $\mu_0 = 3\rho_0(\beta - 1)$, zero subscripts denote evaluation at $x = 0$,

$$H(x) := \frac{2x^2 - (\beta^2\delta + 1 + \gamma)}{2x^2 - (\beta^2\delta + 1 - \gamma)},$$

$$J(x) := 3\beta(\beta - 1)(2 + \delta) + (1 + 6\delta\beta + 9\beta - \beta^2\delta)x^2 - 3(1 + \beta\delta)x^4,$$

$$\gamma := [(\beta^2\delta - 1)^2 - 8\beta^2]^{1/2}.$$

The metric components are

$$A = \text{const. } H^{\beta/\gamma},$$

$$B = \text{const. } F^{-1/2} H^{-\beta^2\delta + 2\beta - 1}/\gamma.$$

Schwarzschild's constant density solution is given for the parameter value $\delta = \beta^{-2} - 3\beta^{-1}$, which lies outside the range of constraint (28).

Finally, upon matching a solution to the exterior Schwarzschild metric and using $B'/B = (e + u)/\rho$, the total mass is given by

$$M = 2\rho_b e_b^{-1} [1 - (1 + e_b^2)^{1/2}]. \quad (29)$$

7. REMARKS

In the new formulation of the spherical equilibrium problem, one starts with an equation of state and then solves the $e-f$ Eq. (19). This is equivalent to the Newtonian case of starting, for instance, with a polytropic equation of state and then solving the Lane-Emden equation. Upon finding an $e-f$ solution, the metric is obtained by quadrature.

In the post-Newtonian approximation, distributions of matter in spherically symmetric hydrostatic equilibrium are governed by the pressure-density equations which arise as coefficients upon expanding the $e-f$ equation

in powers of c^{-2} .

Regarding the Weyl tensor, none of the physically valid solutions considered in this work can be conformally flat, since Collinson⁹ has shown the unique conformally flat static Schwarzschild interior to be Schwarzschild's constant density solution.

Adiabatically stable solutions in closed form are provided by the solution generating technique.

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⁶S. P. Goldman, Master's thesis (University of Windsor, 1977) (unpublished).

⁷In practice, one can avoid integrating Eq. (21) by using $B^2 = (u^2 + 2u - e^2)/(8\pi p \rho^2)$, with Eqs. (18) and (22).

⁸Condition (iii) with $p < \mu$ rather than $p < \frac{1}{3}\mu$ allows the possibility of nongravitational interactions when determining the equation of state.

⁹C. D. Collinson, Gen. Rel. Grav. 7, 419 (1976).

Solitons and the delta function fermion gas in Hartree-Fock theory^{a)}

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The quantum-mechanical, fermion, attractive delta function gas in one dimension has many interesting, known physical properties, including some aspects of soliton behavior. Motivated by a desire to test the validity of the HF approximation to many-body systems, we have made a rigorous study of the HF theory of this gas. When the particle number is even we can show that although HF theory does not give energies accurately, it does correctly predict the known qualitative properties; in particular, only two-particle bound states exist.

I. INTRODUCTION

The Hamiltonian for N particles in one dimension interacting via a delta function potential is

$$H = -\sum_{i=1}^N \Delta_i - 2c \sum_{i < j}^N \delta(x_i - x_j), \quad (1.1)$$

$$\nabla_i = \frac{\partial}{\partial x_i}, \quad \Delta_i = \nabla_i^2. \quad (1.2)$$

Its ground state has several interesting properties and our main purpose will be to investigate the Hartree-Fock (HF) theory of this system for *fermions* to see whether the qualitative features of the exact ground state hold in HF theory. Our motivation is that while HF theory can be shown to exist in many cases, in the sense that the HF equations do have solutions which minimize the HF energy, very little is known rigorously about these solutions, even in the simplest cases. An example is the recent proof¹ that HF theory exists for atomic and molecular systems, but even for the two-electron one-nucleus problem with $Z < 2$ it is not obvious what the HF ground state is. Because the HF equations are highly nonlinear, attempts to solve them on a computer are not insensitive to ones unproved preconceptions about the nature of the solution. Therefore, it may be of some academic interest to note that we can prove rigorously that for the *attractive* case ($c > 0$), the HF approximation to (1.1) is correct in several qualitative respects. The HF energy itself is not very accurate; in fact it is wrong by a factor of 3 in the $c \rightarrow \infty$ limit. The repulsive case is more complicated and we shall have little to say about it, apart from some generalities. In fact there is reason to believe that HF theory is not as good in the repulsive case; e.g., it possibly contradicts (D) below.

By fermions we mean spin- $\frac{1}{2}$ particles obeying the Pauli exclusion principle. The allowed wavefunctions $\psi(x_1, \dots, x_N; \sigma_1, \dots, \sigma_N)$, $x_i \in \mathbb{R}$, $\sigma_i = \pm \frac{1}{2}$, are antisymmetric in every pair (x_i, σ_i) and (x_j, σ_j) . The ground state energy is

$$E_0(N) = \inf \langle \psi, H\psi \rangle / \langle \psi, \psi \rangle, \quad \psi \in L^2. \quad (1.3)$$

We call this the *free case*. If the particles are in a box, $0 \leq x_i \leq L$, we shall denote the energy, defined as in (1.3), by $E_P(N, L)$ or $E_D(N, L)$ if *periodic* or *Dirichlet* ($\psi=0$) boundary conditions are imposed.

Some of the properties of the ground state are:

(A) *Saturation*: If $c \geq 0$, then

$$E(N, \cdot) \geq -c^2 N/4, \quad (1.4)$$

in the Dirichlet or free cases. If $c \leq 0$, then $E(N, \cdot) \geq 0$ in all three cases.

(B) *Thermodynamic limit*: For any c

$$\lim_{N \rightarrow \infty} N^{-1} E_0(N) = e(0) \quad (1.5)$$

exists;

$$\lim_{N \rightarrow \infty} N^{-1} E_P(N, N/\rho) = \lim_{N \rightarrow \infty} N^{-1} E_D(N, N/\rho) = e(\rho), \quad (1.6)$$

exists for all densities $\rho > 0$. Moreover,

$$\lim_{\rho \rightarrow \infty} e(\rho) = e(0), \quad (1.7)$$

and $\rho e(\rho)$, the energy per unit volume, is a convex function of ρ and $e(\rho)$ is a nondecreasing function of ρ . All this is proved in the Appendix.

(C) *There are only two-particle bound states*²: For $c > 0$

$$E_0(N) = E_0(2)[N/2], \quad (1.8)$$

where $[N/2]$ is $N/2$ for N even and $(N-1)/2$ for N odd. More specifically, if the center of mass motion is removed from (1.1) the right side of (1.3) is a minimum if and only if $N=2$. Furthermore, for two particles,

$$E_0(2) = -c^2/2, \quad (1.9)$$

and the ground state wavefunction is

$$\exp(-c|x_1 - x_2|/2) \{ \uparrow \downarrow - \downarrow \uparrow \}, \quad (1.10)$$

i. e., it is a singlet.

(D) *Antiferromagnetism*: In a box the ground state

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wavefunction always exists for any c and a boundary condition. For Dirichlet boundary conditions and any c the ground state wavefunction is nondegenerate and its spin is the lowest value possible,³ i. e., $S=0$ or $\frac{1}{2}$.

(E) *Scaling*: In all cases the dependence on c is such that by changing the length scale: $x \rightarrow |c|x$, the problem reduces to the $|c|=1$ problem. In particular, introducing the c dependence

$$E(N, L; c) = c^2 E(N, |c|L; c/|c|), \quad (1.11a)$$

$$e(\rho; c) = c^2 e(\rho/|c|; c/|c|). \quad (1.11b)$$

Thus $\gamma \equiv c/\rho$, which is dimensionless, is the only non-trivial parameter. In a box $k_F =$ fermi momentum $= \pi\rho/2$, whence $\gamma = \pi c/2k_F$.

Comments: (i) (A) fails dramatically for bosons. If $N \rightarrow \infty$ and $L > l > 0$, l fixed, then² asymptotically (in N)

$$E \sim -c^2 N^3/12, \quad (1.12)$$

and the system collapses. Calogero and Degasperis⁴ investigated the HF theory in the boson case (which is the same as Hartree theory) and showed that HF theory yields the correct asymptotic result (1.12).

(ii) (A) and (C) rest on the assertion⁵: If box boundary conditions are not imposed, it is clear that all solutions of the Schrödinger equation are given by the Bethe ansatz. We do not know a proof of this (except for $N=2$), but shall assume it. The Bethe ansatz yields, by inspection, that the only N -particle bound state is

$$\psi = \exp\left[-\frac{c}{2} \sum_{i < j}^N |x_i - x_j|\right]. \quad (1.13)$$

These are all symmetric, and thus for fermions only the singlet state (1.10) is allowed. Since $E_D(N, L) \geq E_0(N)$, (1.4) holds. In the periodic case there is no bound of the form $E_P(N, L) \geq -\alpha c^2 N$ with α independent of L . To see this, put two particles in the zero momentum state, whence $E_P(2, L) \leq -c/L$. (B) and (C) imply that

$$e(\rho) \geq e(0) = -c^2/4. \quad (1.14)$$

(iii) (B) is proved in the Appendix. It will also be shown there that

$$\begin{aligned} e(\rho) &\leq \pi^2 \rho^2/12 - c\rho/2, & \text{all } \rho \\ e(\rho) &\geq \pi^2 \rho^2/12 - \pi c\rho(12)^{-1/2}, & \rho \geq 3^{1/2}c\pi \\ e(\rho) &\geq -c^2/4, & \rho \leq 3^{1/2}c\pi. \end{aligned} \quad (1.15)$$

The upper bound comes from HF theory. Thus HF theory is asymptotically exact as $\rho \rightarrow \infty$, and we conjecture that the error is not $O(\rho)$, as in (1.15), but only $O(1)$. Cf. (1.40).

(iv) The fact, (D), that the ground state is antiferromagnetic with free or Dirichlet boundary conditions is general.³ It holds in one dimension for any N -body potential. It is far from obvious that it holds in HF theory, however.

Before turning to HF theory we comment on another important and intriguing property of the delta function gas in the free case:

(F) *Only rearrangements can occur in a collision*:

Let us ignore statistics (i. e., symmetry of the wavefunction) and consider the time dependent Schrödinger equation

$$H\psi = \frac{i\partial\psi}{\partial t}. \quad (1.16)$$

As an incoming state take any number of bound complexes of the form (1.13), each with arbitrary particle number and momentum. Then, as shown by McGuire,² there will be no breakup or exchange of momenta. The outgoing state will consist of the same complexes, but with rearrangements of the particles. There will, of course, be phase shifts.

Property (F) is reminiscent of a similar property of solitons.⁶ If one cannot observe which particle is in which complex, then the solutions to the linear equation (1.16) behave just like solitons. The latter occur in nonlinear partial differential equations for a function $\varphi(x, t)$ of one $x \in \mathbb{R}$ and time, for example in the nonlinear Schrödinger equation⁷

$$-\Delta\varphi - 2c|\varphi|^2\varphi = i\frac{\partial\varphi}{\partial t}. \quad (1.17)$$

What, if anything, is the connection between (1.17) and (1.16)? One possibility⁸ is to write H in second-quantized form as

$$H = \int |\nabla\psi(x, t)|^2 dx - c \int [\psi^*(x, t)]^2 [\psi(x, t)]^2 dx.$$

If ψ , which is a quantum field, is replaced by a classical field, then the equation of motion becomes (1.17). This connection is not the one we wish to emphasize. Rather, it is that the time dependent HF equations for (1.16) are a generalization of (1.17) to N coupled equations of the form

$$-\Delta\varphi_j - 2c\rho\varphi_j = \frac{i\partial\varphi_j}{\partial t}, \quad (1.18)$$

where the $\varphi_j(x, t)$ are N orthonormal functions and

$$\rho(x, t) \equiv \sum_{j=1}^N |\varphi_j(x, t)|^2. \quad (1.19)$$

Unfortunately we can say almost nothing about (1.18) when $N > 1$, but if property (F) of the original Schrödinger equation is any guide, (1.18) might be worth further study.

Now we define HF theory. Let

$$\psi = \{\psi_1, \dots, \psi_N\}, \quad (1.20)$$

be a family of N orthonormal, single-particle functions of space and spin, which we write as

$$\psi_i(x, \sigma) = \psi_i^+(x) \uparrow + \psi_i^-(x) \downarrow. \quad (1.21)$$

The ψ_i satisfy one of the three boundary conditions. Define

$$D_\psi \equiv (N!)^{-1/2} \det[\psi_i(x_j, \sigma_j)], \quad (1.22)$$

so that $\langle D_\psi, D_\psi \rangle = 1$. Then

$$\mathcal{E}(\psi) \equiv \langle D_\psi, HD_\psi \rangle = T_\psi^+ + T_\psi^- + U_\psi + K_\psi, \quad (1.23)$$

$$T_\psi^\pm \equiv \sum_{j=1}^N \int |\nabla\psi_j^\pm(x)|^2 dx, \quad (1.24)$$

$$U_\psi \equiv -2c \int \rho_\psi^+(x) \rho_\psi^-(x) dx, \quad (1.25)$$

$$\rho_{\psi}^+(x) \equiv \sum_{j=1}^N |\psi_j^+(x)|^2, \quad (1.26)$$

$$K_{\psi} \equiv 2c \int \left| \sum_{j=1}^N \psi_j^+(x) \psi_j^-(x) \right|^2 dx. \quad (1.27)$$

The HF energy E_0^{HF} , E_P^{HF} , or E_D^{HF} is defined by

$$E^{\text{HF}} = \inf_{\psi} \mathcal{E}(\psi) \geq E. \quad (1.28)$$

A more elegant way to write $U_{\psi} + K_{\psi}$ is to define

$$\rho_{\psi}(x) = \sum_{j=1}^N (\psi_j, \psi_j) = \rho_{\psi}^+(x) + \rho_{\psi}^-(x), \quad (1.29)$$

$$\tau_{\psi}(x) = \sum_{j=1}^N (\psi_j, \sigma \psi_j), \quad (1.30)$$

with $\sigma = (\sigma^x, \sigma^y, \sigma^z)$ and the σ^i are Pauli spin matrices, and where (\cdot, \cdot) is the inner product in spin-space. Then

$$U_{\psi} + K_{\psi} = -(c/2) \int \{ \rho_{\psi}(x)^2 - \tau_{\psi}(x) \cdot \tau_{\psi}(x) \} dx. \quad (1.31)$$

In conventional terminology, $-c \int \rho_{\psi}(x)^2 dx$ is the "direct interaction" and the remainder of (1.31) is the "exchange interaction."

Equations (1.23)–(1.28) define *unrestricted* HF theory because we have not assumed that the ψ_i are real or that they are product functions of space and spin. *Restricted* HF theory is defined by the further restriction that for some integer n_* , $0 \leq n_* \leq N$,

$$\psi_j = f_j(x) \uparrow \quad (1 \leq j \leq n_*), \quad (1.32)$$

$$\psi_j = f_j(x) \downarrow \quad (n_* < j \leq N),$$

$$\langle f_i, f_j \rangle = \delta_{ij} \quad \text{if } 1 \leq i, j \leq n_* \text{ or } n_* < i, j \leq N. \quad (1.33)$$

For the moment we do not assume the f_j are real, but in the next section we will show that they can always be chosen to be real when N is even. (1.23) and (1.26) become

$$\rho_{\psi}^+(x) = \sum_{j=1}^{n_*} |f_j(x)|^2, \quad (1.34)$$

$$\rho_{\psi}^-(x) = \sum_{j=n_*+1}^N |f_j(x)|^2,$$

$$\mathcal{E}(\psi) = \sum_{i=1}^N \int |\nabla f_i(x)|^2 dx - 2c \int \rho_{\psi}^+(x) \rho_{\psi}^-(x) dx. \quad (1.35)$$

In practice, HF theory is usually taken to mean the restricted HF theory. It hardly needs to be said that since $\mathcal{E}(\psi)$ is not quadratic in the ψ_j 's, the restricted and unrestricted theories are not necessarily the same. We will show that they are the same when N is even.

By standard arguments¹, if there is a ψ that actually minimizes the HF energy (1.28), then the ψ_j (of f_j) will satisfy the HF equations. In restricted HF theory these are

$$-\Delta f_j(x) - 2c \rho_{\psi}^-(x) f_j(x) = \epsilon_j f_j(x), \quad j \leq n_* \quad (1.36)$$

$$-\Delta f_j(x) - 2c \rho_{\psi}^+(x) f_j(x) = \epsilon_j f_j(x), \quad j > n_*.$$

In unrestricted HF theory they are

$$-\Delta \psi_j(x, \sigma) - c \rho_{\psi}(x) \psi_j(x, \sigma) + c [\tau_{\psi}(x) \cdot \sigma \psi_j](x, \sigma) = \epsilon_j \psi_j(x, \sigma). \quad (1.37)$$

The ϵ_j , $j \leq n_*$, are the n_* lowest eigenvalues of the linear operator $-\Delta - 2c \rho_{\psi}^-$; a similar statement holds for the remainder of (1.36) and (1.37) (see the Appendix).

If the eigenvalues ϵ_j are replaced by the operator $i\partial/\partial t$, then (1.36) and (1.37) become the time dependent HF equations. If $N=2M$, $n_*=M$ and if $\rho_{\psi}^- = \rho_{\psi}^+$, we recover (1.18) (with M in place of N) from (1.36).

The restricted HF theory (1.35) with periodic boundary conditions was investigated by Overhauser.⁹ One possible choice for the f_j is plane waves; these satisfy (1.36) and the $\rho_{\psi}^{\pm}(x)$ are constant. Conversely, if the $\rho_{\psi}^{\pm}(x)$ are constant, the f_j satisfy (1.36) and must be plane waves; the same is true of (1.37). Overhauser found that for every $c > 0$, and N sufficiently large, there is a choice of the $f_j(x)$ which gives a lower energy $\mathcal{E}(\psi)$ than the plane waves. Thus HF theory breaks the translation invariance of the system. Overhauser did not find the optimum f_j , however.

Our aim will be to prove some facts about HF theory. When $N=2M$ there is obviously some symmetry in the problem and we can make considerable progress in this case. When N is odd we can do very little, but if one is interested only in the thermodynamic limit of the energy (1.5)–(1.7), then even N is sufficient. We will prove the following [cf. (A)–(E) for the exact ground state]:

(A') (A) is true for HF because $E^{\text{HF}} \geq E$.

(B') If the system is in a box, restricted and unrestricted HF theory exist in the sense that there is a ψ that minimizes the HF energy. (B) holds for the HF energy per particle, $e^{\text{HF}}(\rho)$. This is proved in the Appendix.

(G') If N is even, then restricted and unrestricted HF theory are the same in the following strong sense: After a suitable elementary transformation (see Sec. II, after Theorem 1), ψ must be of the form

$$\psi_j = f_j(x) \uparrow, \quad \psi_{j+N/2} = f_j(x) \downarrow, \quad j=1, 2, \dots, N/2 \quad (1.38)$$

with the $f_j(x)$ real. This is Theorem 2.

(C') (C) holds for HF theory if N is even. In the free case and $N=2$ there is a $\psi = \{\psi_1, \psi_2\}$ which minimizes $\mathcal{E}(\psi)$. For any $N > 2$, and $\psi = \{\psi_1, \dots, \psi_N\}$,

$$\mathcal{E}(\psi) > E_0^{\text{HF}}(2)(N/2). \quad (1.39)$$

Thus, for N even,

$$E_0^{\text{HF}}(N) = E_0^{\text{HF}}(2)(N/2), \quad (1.8')$$

and there is no minimizing ψ for $N=2M > 2$. For two particles

$$E_0^{\text{HF}}(2) = -c^2/6. \quad (1.9')$$

The minimizing function is unique except for translations and is of the form (1.32) with $n_*=1$ and

$$f_1(x) = f_2(x) = (c/4)^{1/2} \text{sech}(cx/2). \quad (1.10')$$

This function is a normalized solution of the time independent, nonlinear Schrödinger equation. We cannot prove the absence of odd particle bound states, but conjecture that there are none.

(D') If N is even, then the system is antiferromagnetic by (1.38). Thus, the HF wavefunction D_{ψ} not only

has $S^z=0$ but it also has a definite spin angular momentum $S=0$.

(B') Scaling also obviously holds in HF theory.

We conjecture that the obvious extension of these results to N odd also holds, but we cannot prove it. In particular, in the free case we cannot prove that there is no three-particle bound state in restricted or unrestricted HF theory.

Clearly our main result is (C'). By continuity in L , the very low density gas has $M=N/2$ bumps in the HF density, $\rho_\psi(x)$. We do not know if these are *regularly spaced*. It is tempting to conjecture that they are, and that the bumps remain regularly spaced but flatten out as ρ increases. It is not true, however, that there are bumps for all *finite* N and L , Overhauser's result notwithstanding. As we shall see for $N=2$ and periodic boundary conditions, the plane wave solution is minimal for small L , i. e., $CL \leq \pi^2$. There is no analog of this bifurcation for Dirichlet boundary conditions. What is likely is that for every $N=2M$, M odd, there is a bifurcation of this sort with periodic boundary conditions, but that the critical density at which the bifurcation occurs increases to infinity as N increases. For M even, the bifurcation may *not* occur. We will solve the $N=2$ case completely. For $N=4$ we have a solution (which always has two regularly spaced bumps) which we believe is correct, but we cannot prove this.

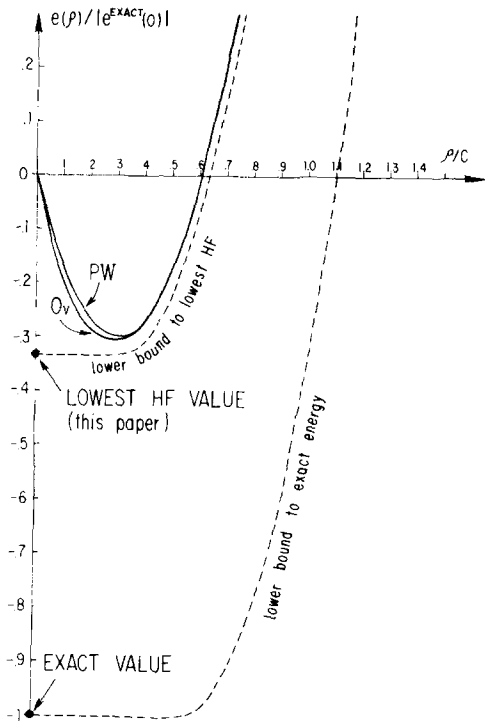


FIG. 1. Ground state energy per particle, in dimensionless units, versus density per unit coupling of the attractive delta interacting one-dimensional fermi gas in various approximations. PW refers to plane wave state, O_V to Overhauser state.⁹ Dashed curves are lower bounds: (1.40) to HF state, and (1.15) to exact ground state. Upper dot is (lowest) HF energy (1.8') and (2.11) found in this paper, while lower dot is exact value (1.7), (1.8), and (1.9).

A final remark concerns the accuracy of E^{HF} . Because of scaling, low density is the strong coupling regime. We see from (1.9) and (1.9') that $E^{HF}/E = \frac{1}{3}$ in this limit. As $\rho \rightarrow \infty$, $E^{HF}/E \rightarrow 1$ [cf. (1.15)]. Parallel to (1.15) there are the following bounds (proved in the Appendix) on the HF energy in the thermodynamic limit:

$$\begin{aligned} e^{HF}(\rho) &\leq \pi^2 \rho^2 / 12 - c\rho / 2, \quad \text{all } \rho, \\ e^{HF}(\rho) &\geq \pi^2 \rho^2 / 12 - \pi\rho c / 6, \quad \rho \geq c/\pi, \\ e^{HF}(\rho) &\geq \sim c^2 / 12, \quad \rho \leq c/\pi. \end{aligned} \quad (1.40)$$

These numerical results, (1.15) and (1.40), together with the Overhauser⁹ result, are shown in Fig. 1. There exists exact results^{10,11} for the ground state energy of this model.

II. PROPERTIES OF HF THEORY

The following establishes (G') and (D').

Theorem 1: Let N be even, $N=2M$. For any boundary conditions the unrestricted HF energy defined by (1.28) is equal to

$$E^R = \inf_{\psi \in \mathcal{R}} \mathcal{E}(\psi), \quad (2.1)$$

where \mathcal{R} is the restricted class of functions of the form (1.38) and with the f_i real.

Proof: Since $K_\psi \geq 0$, and $K_\psi = 0$ when $\psi \in \mathcal{R}$, it is enough to prove that

$$E' \equiv \inf_{\psi} \mathcal{E}'(\psi), \quad (2.2)$$

$$\mathcal{E}'(\psi) \equiv T_\psi^+ + T_\psi^- + U_\psi, \quad (2.3)$$

has the property stated in the theorem. Let ψ be given by (1.21) and ρ_ψ^\pm by (1.26). Regard ρ_ψ^\pm as fixed and define $V_0(x) \equiv \frac{1}{2}[\rho_\psi^+(x) + \rho_\psi^-(x)]$. Then

$$\begin{aligned} \mathcal{E}'(\psi) &= T_\psi^+ + T_\psi^- - 2c \int V_0(x) \rho_\psi(x) dx \\ &\quad + c \int [\rho_\psi^+(x)^2 + \rho_\psi^-(x)^2] dx \end{aligned} \quad (2.4)$$

$$\geq T_\psi^+ + T_\psi^- - 2c \int V_0(x) \rho_\psi(x) dx + 2c \int V_0(x)^2 dx. \quad (2.5)$$

For any real $V(x)$, think of the right side of (2.5), with V_0 replaced by V , as defining a functional $\mathcal{E}_V(\psi)$, and then define $E_V \equiv \inf_{\psi} \mathcal{E}_V(\psi)$. Now since $\psi \rightarrow \mathcal{E}_V(\psi)$ is quadratic, $E_V = E_V^R \equiv \inf_{\psi \in \mathcal{R}} \mathcal{E}_V(\psi)$. This is true if $H_V \equiv -\Delta - 2cV(x)$ has M eigenvalues, $\epsilon_1 \leq \epsilon_2 \leq \dots \leq \epsilon_M$, which satisfy the max-min variational principle; the corresponding eigenfunctions can be chosen to be real, so that $\psi \in \mathcal{R}$ and $E_V = 2 \sum_{j=1}^M \epsilon_j + 2c \int V^2(x) dx$. If H_V does not have eigenvalues, any minimizing sequence $\{\psi^{(n)}\}$, $n=1, 2, \dots$ can obviously be chosen to be in \mathcal{R} . Thus, for any unrestricted ψ ,

$$\mathcal{E}(\psi) \geq \mathcal{E}'(\psi) \geq \mathcal{E}_V(\psi) \geq E_V^R \geq \inf_V E_V^R. \quad (2.6)$$

However, for all ψ and V

$$\begin{aligned} \mathcal{E}_V(\psi) &\geq \inf_V \mathcal{E}_V(\psi) \\ &= \mathcal{E}_{\rho_\psi/2}(\psi) = T_\psi^+ + T_\psi^- - (c/2) \int \rho_\psi(x)^2 dx. \end{aligned} \quad (2.7)$$

If $\psi \in \mathcal{R}$, the latter quantity is $\mathcal{E}(\psi)$, since $\rho_\psi^\pm = \rho_\psi^\pm$. Thus $E_V^R \geq E^R$, for all V . Inserting this in (2.6), the theorem is proved. ■

Remark: We have proved that when $N=2M$, restricted HF theory and unrestricted HF theory (with paired, real functions) agree. We have not proved, however, that one *must take* $\psi \in \mathcal{R}$. There are two reasons for this. One is that if a minimizing ψ does not exist (as it will not in the free case with $M > 1$), then one can have a minimizing sequence in (1.28) with $\psi \notin \mathcal{R}$. The unbound particles will simply "leak away" to infinity and the form of their orbitals is immaterial. The second reason is that we can always make a rotation in spin space so that, for example, \uparrow and \downarrow are replaced by $2^{-1/2}(\uparrow + \downarrow)$ and $2^{-1/2}(\uparrow - \downarrow)$, respectively. Moreover, such a rotation in spin space can be done *independently* for every pair of functions in (1.32) without changing the energy. In fact, it is well known that one can always make the following change in ψ without changing $\mathcal{E}(\psi)$:

Let U be an $N \times N$ unitary matrix. Given ψ , define ψ' by

$$\psi'_i = \sum_{j=1}^N U_{ij} \psi_j. \quad (2.8)$$

Then $\mathcal{E}(\psi) = \mathcal{E}(\psi')$. We shall call a transformation of the form (2.8) an *elementary transformation*. Such transformations also preserve other quantities:

$$\begin{aligned} T_\psi &= T_{\psi'}, \\ \rho_\psi(x) &= \rho_{\psi'}(x), \quad \text{all } x, \\ \tau_\psi(x) &= \tau_{\psi'}(x), \quad \text{all } x. \end{aligned}$$

We can now state the canonical form for ψ when N is even. Essentially, ψ *must* be in \mathcal{R} .

Theorem 2: Suppose $c > 0$, $N=2M$, and ψ is minimizing, i. e., $\mathcal{E}(\psi) = E^{\text{HF}}$. Then, after an elementary transformation, ψ is necessarily of the restricted form (1.38). The functions f_1, \dots, f_M are real, orthonormal, and satisfy

$$\begin{aligned} hf_j &= \epsilon_j f_j, \\ h &\equiv -\Delta - 2c \sum_{j=1}^M f_j(x)^2. \end{aligned}$$

Moreover, $\epsilon_1, \dots, \epsilon_M$ are the M lowest eigenvalues of h .

Remark: The condition $c > 0$ is important. If $c = 0$ and we take periodic boundary conditions on $[0, L]$ and $N = 4$, the following is a minimizing ψ that cannot be brought into the above canonical form:

$$\begin{aligned} \psi_1 &= L^{-1/2} \uparrow, \quad \psi_2 = L^{-1/2} \downarrow, \\ \psi_3 &= L^{-1/2} \exp(ikx) \uparrow, \quad \psi_4 = (2L)^{-1/2} \exp(-ikx) (\uparrow + \downarrow) \end{aligned}$$

with $k = 2\pi/L$.

Proof: The proof of Theorem 1 shows that $K_\psi = 0$. When this statement is put into rotation invariant form, one finds that $\int |\tau_\psi(x)|^2 dx = 0$. Hence $\tau_\psi(x) = 0$, for all x . After an elementary transformation, each ψ_j satisfies (1.37) (with $\tau_\psi = 0$) and the ϵ_j are the M lowest eigenvalues of $h = -\Delta - c\rho_\psi(x)$, each counted twice, of course. The reasons for this are given in section (i) of the Appendix. In the free and Dirichlet cases, the eigenvalues of $-\Delta + V(x)$ are always nondegenerate; in the periodic case an eigenvalue can be at *most* doubly degenerate.

Let the distinct eigenvalues of h be $\epsilon_1 < \epsilon_2 < \epsilon_3$, etc., with at most a double degeneracy for each ϵ_i . We can think of putting the ψ_i into each level in turn. We argue inductively that, as each level is filled, the ψ_i must be of the form (1.38). The difficulty occurs when the last level is two-fold degenerate (four-fold including spin), but there are only two particles to fill it. First, consider a one-fold level. The (spinless) solution f of $hf = \epsilon f$ must be real. The general solution of $h\psi = \epsilon\psi$ is then a linear combination of $f(x)\uparrow$ and $f(x)\downarrow$. After an elementary transformation, any pair of orthonormal solutions can be brought into this form. Therefore, (1.38) always holds for a nondegenerate level. Next, consider a two-fold level, and let two real, orthonormal solutions to $hf = \epsilon f$ be called $f(x)$ and $g(x)$. The four basic functions are $f\uparrow, f\downarrow, g\uparrow, g\downarrow$. If the level has four particles then, after an elementary transformation, the four ψ_i functions can be brought into the form (1.38) with $f_j = f, f_{j+1} = g$.

Finally, consider the case that the last level is two-fold degenerate (four-fold with spin), but there are only two particles left to fill it. The previous $N-2$ ψ_i contribute zero to $\tau_\psi(x)$, i. e., $\sum_{i=1}^{N-2} (\psi_i, \sigma \psi_i)(x) = 0$, by construction. Given a spinor $\alpha = (x, y)$ we define $\hat{\alpha} = (-y^*, x^*)$. If two spinors, α_1 and α_2 , satisfy $(\alpha_1, \sigma \alpha_1) + (\alpha_2, \sigma \alpha_2) = 0$, then $\alpha_2 = \exp(i\theta) \hat{\alpha}_1$, θ real. If we write $\psi_{N-1} = (af(x) + bg(x), cf(x) + dg(x))$ in spinor notation, then ψ_{N-1} is represented by the matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$. Likewise, ψ_N is represented by some matrix B . To say that ψ_{N-1} is of the form $F(x)\alpha$, α a fixed spinor, is to say that A has rank one. An elementary transformation replaces A by $C = sA + tB$ with $|s|^2 + |t|^2 = 1$. We can choose s and t such that C has rank one (by setting $\det C = 0$). Thus, after a preliminary transformation we have $\psi_{N-1} = F(x)\alpha$. By the above remark, ψ_N must be $\psi_N = \exp[i\theta(x)] F(x)\hat{\alpha} \equiv H(x)\hat{\alpha}$, with $\theta(x)$ real. H and F are linear combinations of f and g . There are three cases:

Case 1: $H(x) = \lambda F(x)$, for some λ with $|\lambda| = 1$. By an elementary transformation we can take $\lambda = 1$.

Case 2: $H(x)^* = \lambda F(x)$, $|\lambda| = 1$. Again, take $\lambda = 1$.

Case 3: $H \neq \lambda F$ and $H^* \neq \lambda F^*$. Then $\exp[i\theta(x)] F(x) = H(x)$ and, by complex conjugation, $\exp[i\theta(x)] H^*(x) = F^*(x)$. Thus, $\exp[i\theta(x)]$ maps two independent linear combinations of f and g into linear combinations of f and g . Therefore, $\exp[i\theta(x)] f(x) = R_{11} f(x) + R_{12} g(x)$ and $\exp[i\theta(x)] g(x) = R_{21} f(x) + R_{22} g(x)$. The matrix R must be unitary. Let $\gamma = \exp(i\mu)$, μ real, be an eigenvalue of R , and (p, q) its eigenvector. With $l(x) \equiv pf(x) + qg(x)$, we have $\exp[i\theta(x) - \mu] l(x) = l(x)$. But $l(x)$ is an eigenfunction, so $\exp[i\theta(x)] = \exp(i\mu)$ almost everywhere. Then $H(x) = \exp(i\mu) F(x)$ and we are in Case 1.

Thus far we have proved that the last two orbitals are of the form $\psi_{N-1} = F(x)\alpha$, $\psi_N = H(x)\hat{\alpha}$, and either $H = F$ or $H = F^*$. We will now prove that F must be $\exp(i\theta)G$ with G real. If this is so, the theorem is proved. Write $F(x) = af(x) + ibg(x)$ with f and g real, normalized solutions of $h\psi = \epsilon\psi$ and a, b real. Then $a^2 + b^2 = 1$. Consider the terms in $\mathcal{E}(\psi)$ which depend on ψ_{N-1} and ψ_N . Since $\tau_\psi(x) = 0$, these are

$$B_F = 2 \int |\nabla F|^2(x) dx$$

$$-2c \int |F(x)|^2 \tilde{V}(x) dx - 2c \int |F(x)|^4 dx, \quad (2.9)$$

with $\tilde{V}(x) = 2 \sum_{j=1}^{M-1} f_j(x)^2$. Then

$$\beta_F = a^2 \beta_f + b^2 \beta_j + \delta,$$

with

$$\delta = 2ca^2b^2 \int [f^2(x) - g^2(x)]^2 dx \geq 0.$$

If $a=0$ or $b=0$ there is nothing to prove, so suppose $a \neq 0$, $b \neq 0$, and $\beta_f \leq \beta_g$. There is another possible choice for F and H , namely f and f . This second choice also has $\tau_\psi(x) = 0$. Suppose $\delta > 0$. Then this second choice has a distinctly lower energy than $\mathcal{E}(\psi)$, and we have a contradiction. If $\delta = 0$, then $|f(x)| = |g(x)|$ almost everywhere. Since f and g are real eigenfunctions of h , $f = \pm g$. In this case, $F = \exp(i\theta)f$ and we are done. ■

Having proved that HF theory preserves the antiferromagnetic nature of the system (for N even), we now turn to the second main result of this paper, namely that *there are only 2-body bound states in the free case* (again, N even). The proof is in two parts:

(i) Theorem 3 states that a 2-body state exists and is essentially unique. This means not only that $E_0^{\text{HF}}(2) < 0$ but that there exists a minimizing ψ for $\mathcal{E}(\psi)$. Although it is easy to show that a minimizing ψ always exists in the box case (see the Appendix), it is by no means obvious that a minimizing ψ exists in the free case for *any* N . Indeed, when $N=1$ it never exists (any c), and when $c \geq 0$ it never exists for any N .

(ii) Theorem 4 states that when $N > 2$, including odd N , $\mathcal{E}(\psi)$ is strictly larger than $(N/2)E_0^{\text{HF}}(2)$.

Theorem 3: In the free case, with $N=2$, there exists a minimizing $\psi = \{f(x) \uparrow, f(x) \downarrow\}$, for $\mathcal{E}(\psi)$. This f is unique except for translations, i. e., $f(x) \rightarrow f(x+a)$, and by multiplication by a phase factor, i. e., $f(x) \rightarrow \exp(i\theta)f(x)$, and is given by

$$f(x) = (c/4)^{1/2} \operatorname{sech}(cx/2). \quad (2.10)$$

The HF energy is given by

$$E_0^{\text{HF}}(2) = -c^2/6. \quad (2.11)$$

Proof: By Theorems 1 and 2 we need only consider ψ 's of the above restricted form, even in unrestricted HF theory. Thus, we want to minimize

$$\mathcal{E}(\psi) = W(f) = T + U, \quad (2.12)$$

$$T \equiv 2 \int |\nabla f(x)|^2 dx, \quad (2.13)$$

$$U \equiv -2c \int |f(x)|^4 dx. \quad (2.14)$$

We claim that there is a minimizing f for $W(f)$ subject to $\int |f|^2 = 1$. The only proof we know of this fact is an imitation of the proof for a similar, but more complicated, three-dimensional problem.¹² The steps are: (a) It is sufficient to consider minimization of $W(f)$ subject only to $\int f^2 \leq 1$. (b) By using rearrangement inequalities one shows that if $f(x)$ is not real or not of one sign, then $W(f) > W(|f|)$. Furthermore, f can be assumed to be symmetric decreasing. (c) If $f^{(n)}$ is a minimizing sequence, one can assume $f^{(n)} \rightarrow f$ weakly. Also, $f^{(n)}(x) \rightarrow f(x)$ pointwise by Helly's theorem.¹³ By Sobolev's inequality (cf. the Appendix), $f^{(n)} \in L^2 \cap L^6$ and all the

$f^{(n)}$ are in a fixed ball in $L^2 \cap L^6$; this implies that $f^{(n)}(x) < ax^{-1/2}$ and $f^{(n)}(x) < bx^{-1/6}$. Therefore, $\int [f^{(n)}]^4 \rightarrow \int f^4$ by dominated convergence and $\limsup T(f^{(n)}) \geq T(f)$.

It is a standard fact that any minimizing f satisfies

$$-\Delta f(x) - 2c |f(x)|^2 f(x) = ef(x). \quad (2.15)$$

By Theorem 2, f can be assumed to be real and to be the ground state of $-\Delta - 2cf(x)^2$. Hence $f(x) > 0$, for all x . We can solve (2.15) explicitly by multiplying it by ∇f and integrating. Then

$$(\nabla f)^2 + cf^4 + ef^2 = 0. \quad (2.16)$$

This leads to (2.10) by quadratures, with $e = -c^2/4$ by the normalization of f . ■

Theorem 4: Let $N > 2$ (including odd N). Then for any ψ , $\mathcal{E}(\psi) > (N/2)E_0^{\text{HF}}(2)$.

Remark: Note that ψ is unrestricted.

Proof: As in the proof of Theorem 1 [cf. (2.5), (2.6)] we note that $\mathcal{E}(\psi) \geq \mathcal{E}_V(\psi)$ with $V = (\rho_0^+ + \rho_0^-)/2 \in L^1(\mathbb{R}) \cap L^3(\mathbb{R})$. Consider the Schrödinger operator $H = -\Delta - 2cV(x)$ on $L^2(\mathbb{R})$ and let $\epsilon_1 < \epsilon_2 < \dots < \epsilon_K$ be the negative eigenvalues (if any) of H (K might be infinite). In one dimension, standard Sturm–Liouville theory tells us that ϵ_i is strictly less than ϵ_{i+1} . By the maximum variational principle we have that for any φ ,

$$\mathcal{E}_V(\varphi) \geq 2 \sum_{i=1}^K \epsilon_i + 2c \int V^2 \equiv W, \quad (2.17)$$

and the inequality in (2.17) is strict when $K < N/2$ or $K > N/2$. By Hölder's inequality

$$\sum_{i=1}^K |\epsilon_i| \leq \left[\sum_{i=1}^K |\epsilon_i|^{3/2} \right]^{2/3} K^{1/3}, \quad (2.18)$$

and, since the ϵ_i are distinct, inequality (2.18) is strict if $K \geq 2$. Using the following Lemma 5 and (2.18) we have that

$$\mathcal{E}(\psi) > -2 \left(\frac{3}{16} v \right)^{2/3} (N/2)^{1/3} + v/2c \equiv f(v), \quad (2.19)$$

with $v \equiv (2c)^2 \int V^2$. Thus

$$\mathcal{E}(\psi) > \min_{v \geq 0} f(v) = -Nc^2/12 = (N/2)E_0^{\text{HF}}(2). \quad \blacksquare$$

Lemma 5: Let $U \in L^2(\mathbb{R})$ and let $\epsilon_1 < \epsilon_2 < \dots$ be the negative eigenvalues (if any) of the Schrödinger operator $H = -\Delta - U(x)$ on $L^2(\mathbb{R})$. Let $U_+(x) = U(x)$ if $U(x) \geq 0$ and $U_+(x) = 0$ otherwise. Then

$$\sum_i |\epsilon_i|^{3/2} \leq \frac{3}{16} \int U_+(x)^2 dx, \quad (2.20)$$

with equality if and only if $U = U_+$ and U is reflectionless.

Proof: The lemma is a consequence of the trace formula used in the theory of the Korteweg–de Vries equation,^{14,15}

$$\int_{-\infty}^{\infty} U(x)^2 dx = \frac{16}{3} \sum_i |\epsilon_i|^{3/2} - 4 \int_{-\infty}^{+\infty} k^2 T(k) dk,$$

where $T(k) = \pi^{-1} \ln(1 - |R(k)|^2) \leq 0$ and $R(k)$ is the scattering reflection coefficient for a wave of momentum k . The replacement of U by U_+ in (2.20) follows from the observation that if U is replaced by U_+ , then, by the

max-min variational principle, all the eigenvalues decrease.

To conclude this section we present the solutions to the HF equations in some special cases.

(a) $N=2$, *periodic boundary conditions*: By Theorem 2 there is one common real $f(x)$ which satisfies

$$-f''(x) - 2cf^3 = ef, \quad (2.21)$$

$$E^{HF} = 2e + 2c \int f(x)^4 dx. \quad (2.22)$$

It is convenient to think of (2.21) as a classical equation of motion for a particle with coordinate f in a potential $cf^4 + ef^2$, with $f(0)=f(L)$. Thus $(f')^2 + P(f) = 0$, where $P(f) = cf^4 + ef^2 + \alpha$, $f(x) \geq 0$ since f is the ground state of $-\Delta - 2cf^2(x)$ (see the Appendix). Therefore, $P(f)$ must have two nonnegative zeros $P(f) = c(f^2 - a^2)(f^2 - b^2)$, $a > b \geq 0$. If these two zeros are equal $a=b < 0$, $f(x) = \text{constant}$. The normalization condition then gives in this case

$$f(x) = L^{-1/2}, \quad (2.23)$$

and

$$e = E^{HF} = -2c/L. \quad (2.24)$$

This is the "plane wave" solution to (2.21). Otherwise there are two turning points [the zeros of $P(f)$] and¹⁶

$$f(x) = \omega \operatorname{dn}(\beta x | k), \quad (2.25)$$

where ω , β , k are constants and dn is a Jacobi elliptic function. Since $\operatorname{dn}' = -2 \operatorname{dn}^3 + (2-k) \operatorname{dn}$, one finds that

$$\beta^2 = \omega^2 c, \quad e = (k-2)\beta^2. \quad (2.26)$$

The fundamental period of $\operatorname{dn}(x|k)$ is $2K$, where

$$K = I_{-1/2}, \quad (2.27)$$

with

$$I_p \equiv \int_0^{\pi/2} (1 - k \sin^2 \theta)^p d\theta. \quad (2.28)$$

By a rearrangement inequality f has only one maximum in $(0, L)$, so

$$2K = \beta L. \quad (2.29)$$

Alternatively, this can be seen by setting $\beta L = 2nK$ and then verifying that $n=1$ gives the lowest energy. Finally,

$$1 = \int_0^L f(x)^2 dx = (2\omega^2/\beta) I_{1/2}. \quad (2.30)$$

Thus

$$cL = 4 I_{1/2} I_{-1/2} \equiv \gamma(k), \quad (2.31)$$

$$e = (k-2)c^2 [2I_{1/2}]^{-2}. \quad (2.32)$$

Now $-\infty < k < 1$, and it is easy to see that $\gamma(k)$ is increasing as k goes from zero to one, with $\gamma(1) = \infty$. There is no need to consider $k < 0$, for the substitution $k \rightarrow -k(1-k)^{-1}$ leaves γ unchanged and merely shifts f by half a period. Thus, the solution, (2.25), to (2.21) holds only when

$$cL \geq \gamma(0) = \pi^2, \quad (2.33)$$

and when $k=0$, (2.25) reduces to (2.23). Since $\int_0^K \operatorname{dn}^4 = I_{3/2}$ we have for (2.25)

$$E = (c^2/2)[(k-2)I_{1/2}^{-2} + I_{3/2}I_{1/2}^{-3}]. \quad (2.34)$$

We claim that (2.34) is less than (2.24) for $k > 0$. Using (2.31) this is equivalent to

$$I_{1/2}^2 < I_{-1/2}[(2-k)I_{1/2} - I_{3/2}] \\ = I_{-1/2} \int_0^{\pi/2} (1 - k \sin^2 \theta)^{1/2} (1 - k \cos^2 \theta) d\theta. \quad (2.35)$$

By the Schwarz inequality the right side of (2.35) is greater than $\{\int_0^{\pi/2} (1 - k \cos^2 \theta)^{1/2} d\theta\}^2 \equiv I_{1/2}^2$.

To summarize: The HF solution is

$$cL \leq \pi^2 \text{ (plane waves)} \quad cL \geq \pi^2 \\ e \quad (2.24) \quad (2.32) \\ E^{HF} \quad (2.24) \quad (2.34) \\ f(x) \quad (2.23) \quad (2.25),$$

f is unique except for translations.

In this case there is an interesting bifurcation at $cL = \pi^2$ [the solution (2.23) exists for all L , but it is *not* the minimum when $cL > \pi^2$]. Contrary to what Overhauer found⁹ in the thermodynamic limit, the plane wave solution *can* be the lowest for small coupling. It is also worth noting that a low-lying eigenfunction (not the ground state, however) of the Schrödinger equation has nonanalytic behavior at $cL=4$, at which point the Bethe ansatz does not hold.¹⁷

(b) $N=2$, *Dirichlet boundary conditions*: Since $f(0) = f(L) = 0$ and $f(x) \geq 0$, we must have [following (a)] $P(f) = c(f^2 - a^2)(f^2 - b^2)$, $a > 0$, $b \geq 0$. This yields¹⁶

$$f(x) = -\omega \operatorname{cn}(\beta x + K | k) \quad (2.36)$$

[Note: $f \neq \omega \operatorname{sn}$] and

$$2K = 2I_{-1/2} = \beta L, \quad e = \beta^2(1-2k), \quad \beta^2/\omega^2 = c/k. \quad (2.37)$$

The normalization condition is

$$1 = \int_0^L f(x)^2 dx = (2\omega^2/\beta k) \{(k-1)I_{-1/2} + I_{1/2}\}, \quad (2.38)$$

which implies that $0 < k < 1$ is determined by

$$cL = 4I_{-1/2} \{I_{1/2} - (1-k)I_{-1/2}\}. \quad (2.39)$$

It is easy to check that as k goes from 0 to 1 the right side of (2.39) increases monotonically from 0 to ∞ . Therefore, k and the solution (2.36) is uniquely determined for each L . There is no bifurcation as there is for periodic boundary conditions [case (a)].

(c) $N=4$, *Periodic boundary conditions*: Two functions, f_1 , and f_2 are to be found. Plane waves, namely $f_1(x) = L^{-1/2}$, $f_2(x) = L^{-1/2} \exp(i2\pi x/L)$, satisfy the HF equations (1.36) with $V(x) = \rho_0^*(x) = 2/L$. This choice cannot minimize $\mathcal{E}(\psi)$ however because, by Theorem 2, f_1 and f_2 can always be chosen to be real eigenfunctions of $-\Delta - 2cV(x)$. The functions f_1 and $\tilde{f}_2(x) = (2/L)^{1/2} \cos(2\pi x)$ are such a choice, but then $V(x) = 2/L \neq f_1(x)^2 + \tilde{f}_2(x)^2$, and the HF equations are not satisfied. This remark applies to all cases $N=2M$, M even, and therefore the same bifurcation as in case (a) can occur only when M is odd.

An obvious choice for f_1 and f_2 which satisfies the HF equations is

$$\begin{aligned} f_1(x) &= \omega_1 \operatorname{dn}(\beta x | k), \\ f_2(x) &= \omega_2 \operatorname{cn}(\beta x | k), \end{aligned} \quad (2.40)$$

with $\beta L = 4K$ (not $2K$). We omit the details because we cannot prove that (2.40) is minimizing, but we conjecture that it is. $\rho_0^\pm(x) = f_1(x)^2 + f_2(x)^2$ has two equal bumps,¹⁶ and (2.40) goes over into the correct solutions as $L \rightarrow \infty$ or $L = 0$.

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APPENDIX

Here we sketch the proof of some basic facts which are needed in the main text, particularly (B), (B'), (1.15), and (1.40).

(i) In a box (with either boundary condition) there is a minimizing ψ for $\mathcal{E}(\psi)$ in both the restricted and unrestricted HF theories. Basically, the proof is the following: We take each $\psi_i \in W^1$, i. e., the functions such that $\|f\| \equiv \int |f|^2 < \infty$ and $\|\nabla f\|^2 \equiv \int |\nabla f|^2 < \infty$. If $f \in W^1$, then $f \in L^\infty$ because

$$\begin{aligned} |f(x)|^2 &= \int_{-\infty}^x [f^*(y)(\nabla f)(y) + f(y)\nabla f^*(y)] dy \\ &\leq 2 \left[\int_{-\infty}^x |f(y)|^2 dy \right]^{1/2} \left[\int_{-\infty}^x (\nabla f)^2(y) dy \right]^{1/2} \\ &\leq \|f\| \|\nabla f\|. \end{aligned}$$

Hence $\psi_i \in L^p$, $2 \leq p \leq \infty$ and all the integrals in $\mathcal{E}(\psi)$ make sense. Also $\mathcal{E}(\psi)$ is bounded below; this follows either from the Rayleigh–Ritz principle (A) or from a Sobolev inequality. The basic fact we shall use is the Sobolev imbedding theorem that W^1 of a box is compactly imbedded in L^p , $2 \leq p \leq \infty$. This means that if $\psi^{(n)}$ is a minimizing sequence for $\mathcal{E}(\psi)$, $\mathcal{E}(\psi^{(n)}) \rightarrow E^{\text{HF}}$, then, by passing to a subsequence if necessary, there exists a ψ^∞ such that $\psi_i^{(n)} \rightarrow \psi_i^\infty$ in a L^p norm. The L^2 convergence, in particular, ensures the orthonormality of the ψ_i^∞ . Thus, for all the integrals in $\mathcal{E}(\psi)$ except the kinetic energy, i. e., $\delta(\psi) \equiv \mathcal{E}(\psi) - T_\psi$, we have that $\delta(\psi^{(n)}) \rightarrow \delta(\psi^\infty)$. Furthermore, $f \rightarrow \int |\Delta f|^2$ is lower semicontinuous, so that $\liminf_{n \rightarrow \infty} \mathcal{E}(\psi^{(n)}) \geq \mathcal{E}(\psi^\infty)$. Therefore, ψ^∞ minimizes $\mathcal{E}(\psi)$. The argument that ψ^∞ satisfies the HF equations (1.36) and (1.37) (after an elementary transformation) is standard and simple. The eigenvalues in (1.36) and (1.37) are the lowest eigenvalues of the linear operator $-\Delta - 2c\rho_0^\pm(x)$ because $\mathcal{E}(\psi)$ is quadratic (not quartic!) in each f_j (or ψ_j) [cf. Eq. (1.31)].

(ii) The proof of the existence of the thermodynamic limit for the ground state energy per particle in the Dirichlet case is standard. The same proof works for both the Schrödinger and HF theories. The basic observation is that

$$N^{-1}E_D(N, L) \geq (2N)^{-1}E_D(2N, 2L), \quad (A1)$$

and so $N^{-1}E_D(N, N/\rho)$ is decreasing in N and bounded [by (1.4)], and therefore has a limit. (A1) is proved by dividing the box $[0, 2L]$ into two boxes $[0, L]$ and $[L, 2L]$

and using as a variational function the same N -particle function in each box. No “corridors” are required because the delta function has zero range. The limit of $N^{-1}E_0(N)$ [or $N^{-1}E_0^{\text{HF}}(N)$] in the free case can be proved either by repeating the previous argument or else by using the explicit formulas, given in the text, for these quantities.

The convexity of $\rho e(\rho)$ in ρ is standard and follows from (A1). The monotonicity of $e(\rho)$ comes from the fact that decreasing L raises the kinetic energy; alternatively one can say that Dirichlet functions for one value of L are always Dirichlet functions for any larger L .

(iii) With $e(\rho) \equiv \lim_{N \rightarrow \infty} N^{-1}E_D(N, N/\rho)$ we want to show that

$$\lim_{N \rightarrow \infty} N^{-1}E_P(N, N/\rho) = e(\rho). \quad (A2)$$

Our proof will hold for any statistics. On the one side we have the inequality

$$E_P(N, L) \leq E_D(N, L), \quad (A3)$$

because the Dirichlet functions can be used as variational functions for the periodic case. To establish an inequality in the reverse direction, let g be an infinitely differentiable function on $[0, \infty)$ such that $g(x) = 1$, $x = 0$; $g(x) = 0$, $x \geq l$ for some fixed $l > 0$, and $0 \leq g(x) \leq 1$. Assume $L \geq 2l$ and let $f(x) \equiv 1 - g(x) - g(L - x)$, $F(x) \equiv \prod_{i=1}^N f(x_i)$. Thus, if ψ is periodic, then $\varphi = \psi F$ is Dirichlet. We calculate the variational energy

$$\tilde{E} = \langle \varphi | H | \varphi \rangle / \langle \varphi | \varphi \rangle, \quad (A4)$$

assuming that ψ is a (complex) normalized, periodic ground state of H , $H\psi = E\psi$. A simple integration by parts in the kinetic energy term yields

$$\begin{aligned} \tilde{E} &= E + \langle \varphi | \varphi \rangle^{-1} \sum_{i=1}^N \int |\psi(x_1, \dots, x_N)|^2 \\ &\quad \times [\nabla f(x_i)]^2 \prod_{j \neq i} f^2(x_j) dx_1 \cdots dx_N \\ &\leq E + \int_0^L \rho(x) [\nabla f(x)]^2 dx \langle \varphi | \varphi \rangle^{-1}. \end{aligned} \quad (A5)$$

In the last inequality we have used $|f(x)| \leq 1$ and

$$\rho(x) = \sum_{i=1}^N \int |\psi(x_1, \dots, x_N)|^2 dx_1 \cdots \hat{dx}_i \cdots dx_N. \quad (A6)$$

In these integrals, $\int dx$ includes a summation on the spin variable, and all integrations are over $[0, L]$. Next, we bound $\langle \varphi | \varphi \rangle = \int |\psi|^2 F$, and write $f^2 = 1 - h$, $0 \leq h(x) \leq 1$. Since $\prod_{i=1}^N [1 - h(x_i)] \geq 1 - \sum_{i=1}^N h(x_i)$, we have that

$$\langle \varphi | \varphi \rangle \geq 1 - \int_0^L \rho(x) h(x) dx. \quad (A7)$$

Choose $l = (2\rho)^{-1}$, $\rho = N/L$, and $g(x) = 1 - \sin \pi \rho x$, $0 \leq x \leq l$. Then $(\nabla f)^2(x) = (\pi \rho)^2 h(x)$ and

$$\begin{aligned} I(\psi) &\equiv \int_0^L \rho(x) h(x) dx \\ &= \int_0^l \cos^2 \pi \rho x [\rho(x) + \rho(L - x)] dx. \end{aligned} \quad (A8)$$

$I(\psi) = \frac{1}{2}$ if $\rho(x) = \text{const} = \rho$. $\rho(x)$ need not be constant, however, but consider $\psi_b(x_1, \dots, x_N) = \psi(x_1 + b, \dots, x_N$

+ b) (mod[0, L]). For all b, ψ_b is also a ground state wave function, and $L^{-1} \int_0^L db \rho_b(x) = \rho$, whence $L^{-1} \int I(\psi_b) db = \frac{1}{2}$. Thus, there is some b such that $I(\psi_b) \leq \frac{1}{2}$. Therefore,

$$E_D(N, L) - E_P(N, L) \leq \pi^2 \rho^2. \quad (A9)$$

(A9) and (A3) imply (A2).

A similar argument can be carried out for the HF theory to show that

$$\lim_{N \rightarrow \infty} N^{-1} E_P^{HF}(N, N/\rho) = \lim_{N \rightarrow \infty} N^{-1} E_D^{HF}(N, N/\rho) \equiv e^{HF}(\rho). \quad (A10)$$

Replace each periodic $\psi_i(x, \sigma)$ by $\varphi_i(x, \sigma) = \psi_i(x, \sigma) f(x_i)$. The φ_i are still single particle functions as required by HF theory. They will not be orthonormal, however, but this defect is easily remedied by letting $D_\varphi = (N!)^{-1/2} \times \det[\varphi_i(x_j, \sigma_j)]$ and estimating $\langle D_\varphi, HD_\varphi \rangle / \langle D_\varphi, D_\varphi \rangle$ as in the Schrödinger case. We omit the details.

(iv) We want to show that

$$\lim_{\rho \rightarrow 0} e(\rho) = e(0), \quad (A11)$$

both in the Schrödinger and HF theories. The left side of (A11) exists because $e(\rho)$ is monotone in ρ . On the one hand, $E_D(N, L) \geq E_0(N)$ by the variational principle, so $\lim_{\rho \rightarrow 0} e(\rho) \geq e(0)$. Now let $\epsilon > 0$ and, in the Schrödinger theory, approximate the two-particle ground state, ψ , given by (1.10), by an infinitely differentiable function φ of compact support (i. e., $\varphi(x_1, x_2; \sigma_1, \sigma_2) = 0$ if $|x_1| > b$ or $|x_2| > b$) such that $\langle \varphi, H\varphi \rangle / \langle \varphi, \varphi \rangle = E_0(2) + \epsilon$. Let $N = 2M$ and let

$$\begin{aligned} \psi(x_1, \dots, x_N; \sigma_1, \dots, \sigma_N) \\ = \varphi(x_1, x_2; \sigma_1, \sigma_2) \varphi(x_3 + 2b, x_4 + 2b; \sigma_3, \sigma_4) \\ \dots \varphi(x_{N-1} + Nb, x_N + Nb; \sigma_{N-1}, \sigma_N). \end{aligned}$$

Then $\langle \psi, H\psi \rangle / \langle \psi, \psi \rangle = (N/2) \{E_0(2) + \epsilon\}$. (Actually, ψ should be antisymmetrized, but this will not affect the conclusion because the delta function has zero range.) Since ψ is also a Dirichlet function for any box with $L \geq Nb$, and since $e(0) = E_0(2)/2$, we have that $\lim_{\rho \rightarrow 0} e(\rho) = e(0) + \epsilon/2$. Letting $\epsilon \rightarrow 0$ proves (A11). The same proof works for HF theory by choosing the approximating two-particle φ to be of the form

$$\begin{aligned} \varphi(x_1, x_2; \sigma_1, \sigma_2) \\ = g(x_1)g(x_2)f(x_1)f(x_2)\{\uparrow\downarrow - \downarrow\uparrow\} \end{aligned}$$

with $f(x)$ given by (1.10') and $g(x)$ an infinitely differentiable function with support $[-b, b]$. This choice preserves the single particle nature of the HF variational function.

(v) *Bounds on the energy:* In a box the kinetic energy operator $T = -\sum_j \Delta_j$ is bounded below by its lowest eigenvalue which, for large N and fixed density ρ is

$$T \geq N\pi^2 \rho^2 / 12. \quad (A12)$$

The state that gives (A12) is a determinant (spin zero),

and we can use it as a variational function. Thus

$$e(\rho) \leq e^{HF}(\rho) \leq \pi^2 \rho^2 / 12 - c\rho / 2. \quad (A13)$$

To obtain a *lower* bound in Schrödinger theory we write $H = T + W = [\lambda T + W] + (1 - \lambda)T$, $0 \leq \lambda \leq 1$, $W = -2c \sum_{i < j}^N \delta(x_i - x_j)$. The first term is bounded by its ground state energy in the free case which is, for large N [cf. (1.8) and (1.9)], $-c^2 N(4\lambda)^{-1}$. The second term is bounded by using (A12). Thus

$$e(\rho) \geq -c^2(4\lambda)^{-1} + (1 - \lambda)\pi^2 \rho^2 / 12. \quad (A14)$$

The same argument applies to HF theory, except that $c^2/4$ is replaced by $c^2/12$ [cf. (1.8') and (1.9')],

$$e^{HF}(\rho) \geq -c^2(12\lambda)^{-1} + (1 - \lambda)\pi^2 \rho^2 / 12. \quad (A15)$$

Maximizing (A14) and (A15) with respect to λ yields

$$e(\rho) \geq \pi^2 \rho^2 / 12 - \pi c \rho (12)^{-1/2}, \quad \rho \geq 3^{1/2} c / \pi, \quad (A16)$$

$$e(\rho) \geq -c^2 / 4, \quad \rho \leq 3^{1/2} c / \pi,$$

$$e^{HF}(\rho) \geq \pi^2 \rho^2 / 12 - \pi c \rho / 6, \quad \rho \geq c / \pi, \quad (A17)$$

$$e^{HF}(\rho) \geq -c^2 / 12, \quad \rho \leq c / \pi.$$

These results were given in the main text, (1.15) and (1.40). It is noteworthy that (A17) and (A13) are extremely close when $\rho \geq c/\pi$.

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Local supersymmetry in (2+1) dimensions. I. Supergravity and differential forms

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The theory of supergravity in (2+1) dimensions, both with and without a cosmological term, is presented. In the latter case, we discover a manifold that has torsion but no curvature. We make extensive use of differential forms and the dimensionality of our space-time allows us to use $SL(2, R)$ spinors. Our results enable us to discuss in an accompanying paper an action describing the theory of a spinning membrane.

I. INTRODUCTION

There has recently been considerable activity in the study of local supersymmetry.¹ Although the major motivation has been towards constructing a renormalizable theory of gravity, supersymmetry has also played an important role in spaces of lower dimensionality. Indeed, one-dimensional "supergravity" coupled to matter may be used to describe the spinning particle² and the analogous theory in two dimensions describes the spinning string,³ which corresponds, when quantized, to the dual models of Neveu-Schwarz⁴ and Ramond.⁵ In one dimension, pure "gravity" is clearly trivial whilst in two dimensions, the Einstein Lagrangian is a divergence and the Rarita-Schwinger action for a vector-spinor field identically zero. In three dimensions, however, neither of these statements is true and this leads us to consider theories of two-dimensional extended systems (membranes) possessing more complicated actions than the volume element analogue of the relativistic string⁶ (or its supersymmetric counterpart). In fact, there seem to be a number of physically distinct actions, all of which may be cast into the form of three-dimensional field theories, and we discuss these in more detail in an accompanying paper Ref. 7.

Since the membrane actions that we shall discuss in II require the theory of three-dimensional supergravity, the remainder of this paper is devoted to the matter free case. We feel that supergravity in three dimensions has its own intrinsic interest, particularly since we can no longer use Majorana spinors (we consider only simple supersymmetry) and it is not obvious, *a priori*, that the theory should be similar to its four-dimensional counterpart. We have also found that differential forms may be used to great advantage and in the next section we give a brief survey of these techniques, together with a summary of useful formulae for $SL(2, R)$ spinors, which we use throughout.

II. DIFFERENTIAL GEOMETRY

In this section we present our notations and outline the essentials for the differential geometry required in our analysis. The use of the exterior calculus of differential forms is widely appreciated by geometers and a physicist's eye view is given in Ref. 8 which also includes application to extended systems and detailed references to the mathematical literature.

Throughout our work we assume that we are dealing

with a three-dimensional C^∞ manifold endowed with a metric g of signature +1 and a connection ω . A general tangent vector field may be written

$$v = v^i \partial_i \quad (2.1)$$

and a general co-vector field may be written

$$\rho = \rho_i e^i, \quad (2.2)$$

where e^i is a basis set of 1-forms and ∂_i the corresponding dual basis

$$e^i(\partial_j) = \delta_j^i. \quad (2.3)$$

We can regard the components v^i as a set of 0-forms which transform under $A \in GL(3, R)$ according to the rule

$$v^i - v'^i = A^i_j v^j. \quad (2.4)$$

The connection allows us to covariantly exterior differentiate these 0-forms as

$$Dv^i = dv^i + \omega^i_j v^j, \quad (2.5)$$

where d denotes ordinary exterior differentiation and the connection 1-forms ω^i_j transform inhomogeneously under a $GL(3, R)$ transformation;

$$\omega'^i_k A^k_j = A^i_k \omega^k_j - dA^i_j. \quad (2.6)$$

The restriction to 0-forms may be removed by replacing the ordinary product $\omega^i_j v^j$ in (2.5) by the exterior product $\omega^i_j \wedge v^j$ if v^j is a vector-valued p -form. We may extend the concept of exterior covariant differentiation to any field transforming under a representation of $GL(3, R)$ and furthermore we impose the condition of metricity on the connection;

$$Dg_{ij} = 0, \quad (2.7)$$

where

$$g = g_{ij} e^i \otimes e^j,$$

i.e., g_{ij} is a tensor-valued 0-form. The presence of a metric allows one to introduce throughout the manifold a field of orthonormal frames e^a , and we have

$$g(e^a, e^b) = \eta^{ab} = \text{diag}(-1, +1, +1) \quad (2.8)$$

and

$$Dg_{ab} = D\eta_{ab} = 0 \Rightarrow \omega_{ab} = -\omega_{ba}. \quad (2.9)$$

To obtain ω^a_b from the connection components $\Gamma^\mu_{\rho\nu}$ expressed in terms of a coordinate basis we need only use (2.6):

$$e_b^\nu \omega_\nu^\mu = e_a^\mu \omega_b^a - de_b^\mu, \quad (2.10)$$

where e_μ^a is the conventional vierbein ($e_\mu^a e_{\nu a} = g_{\mu\nu}$) (more precisely dreibein here) and

$$\omega_\nu^\mu = \Gamma^\mu_{\rho\nu} dx^\rho. \quad (2.11)$$

Clearly, we remain in an orthonormal basis if we restrict the $GL(3, R)$ transformations to belong to the subgroup $SO(2, 1)$. Since $SO(2, 1)$ is a three-parameter group it is convenient to introduce a one-index set of 1-forms, ω^a , related to the two-index set by

$$\omega^a = -\frac{1}{2} \epsilon^a_{bc} \omega^{bc} \quad (2.12)$$

where Latin indices a, b, \dots are elevated by means of the orthonormal metric η^{ab} and ϵ^{abc} is the alternating symbol ($\epsilon^{012} = +1$).

A general p -form field, ϕ , occurring in our theory will transform under a representation of $SO(2, 1)$ near the identity according to

$$\delta\phi = l^a S_a \phi \quad (2.13)$$

where

$$[S_a, S_b] = -\epsilon_{ab}^c S_c. \quad (2.14)$$

The exterior covariant derivative then takes the form

$$D\phi = d\phi + \omega^a \wedge S_a \phi. \quad (2.15)$$

The eight forms $1, e^a, e^a \wedge e^b$ ($a < b$), $e^a \wedge e^b \wedge e^c$ generate the exterior algebra in the cotangent space of our manifold and their Hodge duals are given by

$$\begin{aligned} \epsilon^{abc} &= *(e^a \wedge e^b \wedge e^c) \equiv \text{dual of } (e^a \wedge e^b \wedge e^c), \\ \epsilon^{ab} &= e^c \epsilon_c^{ab} = *(e^a \wedge e^b), \\ \epsilon^a &= \frac{1}{2} e^b \wedge e_b^a = *(e^a), \\ \epsilon &= \frac{1}{3} e^a \wedge e_a = *(1). \end{aligned} \quad (2.16)$$

The ϵ forms satisfy the following algebraic identities:

$$\begin{aligned} e^a \epsilon_{abc} &= \delta_c^a \epsilon_{ab} + \delta_b^a \epsilon_{ac} + \delta_a^a \epsilon_{bc}, \\ e^c \wedge \epsilon_{ab} &= \delta_b^c \epsilon_a - \delta_a^c \epsilon_b, \\ e^b \wedge \epsilon_a &= \delta_a^b \epsilon. \end{aligned} \quad (2.17)$$

We also observe that ϵ is essentially the volume element for our space:

$$\epsilon = (1/3!) \epsilon_{abc} e^a \wedge e^b \wedge e^c = (1/3!) \epsilon_{abc} e_\mu^a e_\nu^b e_\rho^c dx^\mu \wedge dx^\nu \wedge dx^\rho$$

or

$$\epsilon = e dx^0 \wedge dx^1 \wedge dx^2 \quad (2.18)$$

where

$$e = \det e_\mu^a = (-\det g_{\mu\nu})^{1/2}.$$

We define the torsion 2-form, T^a , by

$$T^a = D e^a = de^a + \epsilon_b^a \wedge \omega^b = \frac{1}{2} T^a_{bc} e^b \wedge e^c \quad (2.19)$$

and the curvature 2-form, F^a , by

$$D^2 \phi = S_a F^a \wedge \phi \quad (2.20)$$

$$F^a = \frac{1}{2} F^a_{bc} e^b \wedge e^c$$

$$F^a = d\omega^a - \frac{1}{2} \epsilon^a_{bc} \omega^b \wedge \omega^c. \quad (2.21)$$

F^a is related to the normal two-index curvature 2-form, R^a_b , by

$$F^a = -\frac{1}{2} \epsilon^a_{bc} R^{bc} \quad (2.22)$$

$$R^a_b = \frac{1}{2} R^a_{bcd} e^c \wedge e^d.$$

By exterior differentiation of the definitions (2.19) and (2.21) one obtains the Bianchi identities:

$$DT^a = -\epsilon^a_b \wedge F^b \quad (2.23)$$

$$DF^a = 0.$$

We shall find it useful to employ in some of our manipulations the concept of interior multiplication.^{8,9} Suppose X is a tangent vector field and ϕ a p -form, then we define left interior multiplication⁹ by

$$X \lrcorner \phi = X^a \phi_{bc} \dots \partial_a \lrcorner (e^b \wedge e^c \dots), \quad (2.24)$$

where

$$\partial_a \lrcorner (e^b \wedge e^c \wedge \dots) = \delta_a^b e^c \wedge \dots - \delta_a^c e^b \wedge \dots + \dots. \quad (2.25)$$

Let us illustrate our formalism by a simple example—free gravity in three dimensions. The action is

$$S = \int e^a \wedge F_a \equiv \int \Lambda. \quad (2.26)$$

Since e^a is a 1-form and F^a is a 2-form, Λ is a scalar-valued 3-form and so may be integrated over an oriented 3-chain⁸ to give a reparameterization-invariant action. To obtain the equations of motion we vary the frames, e^a , and the connection, ω^a , independently. The frame variation gives us immediately

$$F^a = 0 \quad (2.27)$$

whilst

$$\delta F^a = d(\delta\omega_a) - \epsilon_{abc} \omega^b \wedge \delta\omega^c.$$

Since

$$e^a \wedge d(\delta\omega_a) = de^a \wedge \delta\omega_a - d(e^a \wedge \delta\omega_a)$$

we obtain

$$\delta\Lambda = \delta e^a \wedge F_a + (de^a + \epsilon^a_b \wedge \omega^b) \wedge \delta\omega_a - d(e^a \wedge \delta\omega_a). \quad (2.28)$$

The last term is an exact form and can at most affect the boundary conditions of the manifold under consideration. Using (2.19), the $\delta\omega^a$ variation therefore gives

$$T^a = 0. \quad (2.29)$$

Thus, the only solution to the Einstein–Cartan theory in empty 3-space is Minkowski space. This is not surprising in view of the fact that the conventional Einstein equations in empty space are

$$K_{\mu\nu} = 0, \quad (2.30)$$

where $K_{\mu\nu}$ is the Ricci tensor, and we note that the 6 independent components of the curvature tensor are therefore uniquely determined by it.

For completeness, let us show that our action (2.26) is indeed the conventional Einstein action. Using the definition (2.20) we have

$$\Lambda = \frac{1}{2} e^a \wedge e^b \wedge e^c F_{abc}.$$

But $e^a \wedge e^b \wedge e^c = \epsilon^{abc} \epsilon$.

Hence

$$\begin{aligned} \Lambda &= \frac{1}{2} \epsilon \epsilon^{abc} F_{abc} \\ &= -\frac{1}{4} \epsilon \epsilon^{abc} \epsilon_{adf} R^{df}{}_{bc} \end{aligned}$$

from (2.22). Using $\epsilon^{abc} \epsilon_{adf} = \delta_f^a \delta_d^b - \delta_f^b \delta_d^a$ and the antisymmetry of R^{ab} on both pairs of indices, we finally obtain

$$\Lambda = \frac{1}{2} \epsilon R^{ab}{}_{ab} = \frac{1}{2} \epsilon R.$$

So

$$S = \int \frac{1}{2} d^3x e R \quad (2.31)$$

where in the final step we have used (2.18).

Since we intend to supersymmetrize this action, we conclude this section with a brief survey of the spinors we shall use. The covering group of $SO(2, 1)$ is $SL(2, R)$ [isomorphic to $SU(1, 1)$] and hence we may utilize real two component spinors. The generators of $SL(2, R)$ satisfy (2.14) and may be realized by the matrices $\frac{1}{2} \gamma_a$ where

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.32)$$

These matrices also provide a realization of the Clifford algebra in three dimensions,

$$[\gamma_a, \gamma_b]_+ = 2\eta_{ab} \quad (2.33)$$

For any two-component spinor, ψ , we define its adjoint, $\bar{\psi}$, by

$$\bar{\psi} = \psi^T \gamma^0 \quad (2.34)$$

and we have only two bilinear invariants

$$\bar{\psi} \psi \quad (\text{pseudoscalar})$$

and

$$\bar{\psi} \gamma_a \psi \quad (\text{vector}).$$

The exterior covariant derivative of a spinor valued p -form ψ is given according to (2.15) by

$$D\psi = d\psi + \frac{1}{2} \gamma_a \omega^a \wedge \psi. \quad (2.35)$$

The virtue of using orthonormal frames is particularly apparent here, since we can always use the constant γ matrices (2.32). Finally, we shall also require the components of our spinors to mutually anticommute (i. e., to be odd elements of some Grassmann algebra) and for any two such spinors we have

$$\begin{aligned} \bar{\psi}_1 \psi_2 &= -\bar{\psi}_2 \psi_1, \\ \bar{\psi}_1 \gamma_a \psi_2 &= -\bar{\psi}_2 \gamma_a \psi_1 \end{aligned} \quad (2.36)$$

while for any three spinors of the above type, we have the Fierz re-arrangement formula

$$(\bar{\psi}_1 \psi_2) \psi_3 = -\frac{1}{2} \sum_A (\bar{\psi}_1 \gamma_A \psi_3) \gamma^A \psi_2 \quad (2.37)$$

$$\gamma_A = 1, \gamma_a; \quad \gamma^A = 1, \gamma^a.$$

III. FREE SUPERGRAVITY IN THREE DIMENSIONS

In the usual approach to supergravity one takes the

basic fields to be the vierbein e_μ^a and the Rarita-Schwinger vector-spinor field χ_μ . In our language these are replaced by the frames themselves and a spinor-valued 1-form χ . The relation between these variables is

$$e^a = e_\mu^a dx^\mu, \quad \chi = \chi_\mu dx^\mu. \quad (3.1)$$

We take as our action the sum of the free gravity action (2.26) and the Rarita-Schwinger action for a vector spinor. The Lagrangian 3-form Λ is then given by

$$\Lambda = e^a \wedge F_a + (i/2) \bar{\chi} \wedge D\chi, \quad (3.2)$$

where $D\chi$ is given by (2.35).

To obtain the equations of motion, we vary the frames, the connection and the spinor 1-form, χ , independently. The variation of $D\chi$ is given by

$$\begin{aligned} \delta(D\chi) &= \delta(d\chi) + \frac{1}{2} \gamma_a \omega^a \wedge \delta\chi - \frac{1}{2} \gamma_a \chi \wedge \delta\omega_a \\ &= D(\delta\chi) - \frac{1}{2} \gamma_a \chi \wedge \delta\omega_a. \end{aligned} \quad (3.3)$$

Hence, the total variation is

$$\begin{aligned} \delta\Lambda &= \delta e^a \wedge F_a + i \delta \bar{\chi} \wedge D\chi + [T^a - (i/4) \bar{\chi} \gamma_a \wedge \chi] \wedge \delta\omega_a \\ &\quad + \text{an exact form.} \end{aligned} \quad (3.4)$$

The equations of motion are therefore

$$F^a = 0, \quad T^a = (i/4) \bar{\chi} \gamma^a \wedge \chi, \quad D\chi = 0. \quad (3.5)$$

It is a characteristic feature of this "first-order" formalism¹⁰ that only two of these equations have dynamical content, the torsion equation being an algebraic one which allows us to solve for ω in terms of the frames and χ . We can decompose the connection ω into a torsion-free part, $\hat{\omega}$, and an additional part, the contortion 1-form, λ^a_b . The torsion-free part, $\hat{\omega}$, corresponds to the usual Christoffel connection via equation (2.10) while from (2.19)

$$T^a = \lambda^a_b \wedge e^b. \quad (3.6)$$

We may solve (3.6) to obtain the components of λ^a_b in terms of the components of T^a :

$$2\lambda_{abc} = T_{cab} - T_{abc} - T_{bca}, \quad (3.7)$$

where

$$T_{abc} = (i/2) \bar{\chi}_b \gamma_a \chi_c, \quad \text{from (3.5).}$$

The equations of motion (3.5) tell us that our manifold has zero curvature but nonvanishing torsion. However, this is not sufficient for the space to be flat. Indeed, both curvature and torsion are connection-dependent quantities and we are free to use $\hat{\omega}$ to define a covariant differential \hat{D} in place of the full ω occurring in the Lagrangian (3.2). In this case, the torsion associated with $\hat{\omega}$ is zero but the curvature is not and the χ equation of motion becomes

$$\hat{D}\chi + \frac{1}{2} \gamma_a \lambda^a \wedge \chi = 0, \quad (3.8)$$

where

$$\lambda^a = -\frac{1}{2} \epsilon^a{}_{bc} \lambda^{bc}.$$

Equation (3.8) corresponds to a nonminimal coupling of a vector-spinor field to conventional (torsion-free) Einstein gravity. Before exhibiting the supersymmetry of our action, we observe that the theory is consistent

(no acausal propagation for χ) despite the appearance of the entire curvature tensor in (3.5). Indeed,

$$D^2\chi = \frac{1}{2}\gamma_a F^a \wedge \chi \quad \text{but} \quad F^a = 0. \quad (3.9)$$

Let us now show that the Lagrangian (3.2) is supersymmetric on the manifold defined by (3.8). We take our transformations to be

$$\delta e^a = i\bar{\alpha}\gamma^a\chi, \quad \delta\chi = 2D\alpha, \quad (3.10)$$

where α is a spinor-valued 0-form. Under (3.10), we find

$$\delta\Lambda = i\bar{\alpha}\gamma^a\chi \wedge F_a + 2iD\bar{\alpha} \wedge D\chi + (T^a - \frac{1}{4}i\bar{\chi}\gamma^a\chi) \wedge \delta\omega_a + \text{an exact form.} \quad (3.11)$$

Now,

$$D\bar{\alpha} \wedge D\chi = d(\bar{\alpha}D\chi) - 2i\bar{\alpha}D^2\chi.$$

But

$$D^2\chi = \frac{1}{2}\gamma^a F_a \wedge \chi$$

from (2.20). Hence the first two terms in (3.11) combine to give an exact form and we are left only with a term which vanishes when we pass to the "second-order" formalism. We therefore conclude that the action corresponding to (3.2) is indeed supersymmetric providing (3.8) holds true.

IV. INCLUSION OF A COSMOLOGICAL TERM

It has recently been shown¹¹ in four dimensions that one can extend supergravity to include a cosmological term if one also adds a mass-like term for the χ field. In this section we show that a similar modification in our action enables us to incorporate a cosmological term. The inclusion of this term is more than an academic exercise. We show in (II) that such a term plays a crucial role in providing a physical interpretation for a system of self-gravitating (super) matter. The action is

$$S = \int e^a \wedge F_a + \frac{i}{2}\bar{\chi} \wedge D\chi - \epsilon + \frac{i}{4}\bar{\chi} \wedge \gamma \wedge \chi \equiv \Lambda, \quad (4.1)$$

where $\gamma = \gamma_a e^a$ is an $SL(2, R)$ algebra-valued 1-form and ϵ is defined in (2.16). Variation yields

$$\delta\Lambda = \delta e^a \wedge (F_a - \epsilon_a + \frac{1}{4}i\bar{\chi} \wedge \gamma_a \chi) + (T^a - \frac{1}{4}i\bar{\chi} \wedge \gamma^a \wedge \chi) \delta\omega_a + i\delta\bar{\chi} \wedge (D\chi + \frac{1}{2}\gamma \wedge \chi) + \text{an exact form.}$$

The equations of motion are therefore

$$F_a = \epsilon_a - T_a, \quad (4.2)$$

$$D\chi + \frac{1}{2}\gamma \wedge \chi = 0,$$

$$T^a = \frac{1}{4}i\bar{\chi} \wedge \gamma^a \chi. \quad (4.3)$$

We observe that this modification is enough to provide curvature, and, indeed, the inclusion of a cosmological term for free gravity is sufficient to make that theory nontrivial.

We take as our supersymmetry transformations the amended form of (3.10)

$$\delta e^a = i\bar{\alpha}\gamma^a\chi, \quad \delta\chi = 2D\alpha + \gamma\alpha. \quad (4.4)$$

With these specific variations and using the defining

equation for the connection (4.3) we find, in addition to the terms occurring (3.11), a piece

$$\bar{\delta}\Lambda = -i\bar{\alpha}\gamma^a\chi \wedge (\epsilon_a - T_a) + iD\bar{\alpha} \wedge \gamma \wedge \chi - i\bar{\alpha}\gamma \wedge D\chi - (i/2)\bar{\alpha}\gamma \wedge \gamma \wedge \chi. \quad (4.5)$$

The second and third terms may be re-arranged to give an exact form plus a term involving the torsion (this arises from transferring the D onto γ). The two terms involving the torsion sum up to give a contribution [upon using (4.3)]

$$-\frac{1}{2}i\bar{\alpha}\gamma^a\chi \wedge (\chi \wedge \gamma_a \chi). \quad (4.6)$$

However, a Fierz re-arrangement (2.37) shows that this term is in fact zero and we are left with

$$-i\bar{\alpha}\gamma^a\chi \wedge \epsilon_a - (i/2)\bar{\alpha}\gamma \wedge \gamma \wedge \chi. \quad (4.7)$$

But

$$\begin{aligned} \gamma \wedge \gamma &= \gamma_{[a}\gamma_{b]}e^a \wedge e^b \\ &= -\epsilon_{abc}\gamma^c e^a \wedge e^b \\ &= -2\gamma^a \epsilon_a \end{aligned} \quad (4.8)$$

using (2.16). Hence, these two terms cancel and the action (4.1) is therefore locally supersymmetric.

We conclude by showing that the algebraic structure of the invariances possessed by our action closes in a field-dependent sense. In our language, an infinitesimal coordinate transformation on a set of differential forms corresponds to a change in the field by a diffeomorphism induced by a vector field. Specifically, if ξ is the vector field,

$$\delta_\xi e^a \equiv \mathcal{L}_\xi e^a, \quad (4.9)$$

where $\mathcal{L}_\xi e^a$ is the Lie derivative of e^a with respect to the vector field ξ . In terms of interior multiplication (2.24) and (2.25),

$$\mathcal{L}_\xi e^a = \xi \lrcorner de^a + d(\xi \lrcorner e^a). \quad (4.10)$$

By re-arranging the terms in (4.10) with the use of the definition of torsion one obtains,

$$\mathcal{L}_\xi e^a = \xi \lrcorner T^a + D\xi^a - \epsilon^a_{bc}(\xi \lrcorner \omega^c)e^b. \quad (4.11)$$

For ordinary supergravity, the transformations (3.10) give

$$[\delta_\beta \delta_\alpha]e^a = D\xi^a, \quad (4.12)$$

where

$$\xi^a = 2i\bar{\alpha}\gamma^a\beta.$$

Hence, using (4.3) and the identity, valid for any two 1-forms, ω and ρ ,

$$\xi \lrcorner (\rho \wedge \sigma) = (\xi \lrcorner \rho)\sigma - (\xi \lrcorner \sigma)\rho \quad (4.13)$$

we find

$$[\delta_\beta \delta_\alpha]e^a = \mathcal{L}_\xi e^a - (i/2)(\xi \lrcorner \bar{\chi})\gamma^a\chi + \epsilon^a_{bc}(\xi \lrcorner \omega^c)e^b. \quad (4.14)$$

The first term is an infinitesimal coordinate transformation, the second a field-dependent supergauge transformation with parameter $\alpha' = -\frac{1}{2}\xi \lrcorner \chi$, and the third an $SO(2, 1)$ transformation with parameter $l^a = \xi \lrcorner \omega^a$. In common with the four-dimensional case,¹² in order to close the algebra on the χ field it is necessary for

the equations of motion (3.5) to be satisfied. In this case $\delta\omega^a = 0$ and hence

$$[\delta_\beta \delta_\alpha] \chi = 0. \quad (4.15)$$

To be consistent with (4.14) we require

$$[\delta_\beta \delta_\alpha] \chi = \mathcal{L}_\xi \chi - D(\xi \lrcorner \chi) + \frac{1}{2}(\xi \lrcorner \omega^a) \gamma_a \chi. \quad (4.16)$$

A short calculation shows that the right-hand side of (4.16) is $\xi \lrcorner D\chi$ and hence vanishes when (3.5) is satisfied. The modification in the transformations for the cosmological case does not alter the basic structure of (4.14), although the additional term in $\delta\chi$ changes the $SO(2, 1)$ parameter by a factor $-\xi^a$. The corresponding change for the χ field comes about from the modification of $\delta\omega$ due not only to (4.4) but also to the χ equation of motion in (4.2).

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Complex line bundles in relativity

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We exhibit the complexified spin and conformally weighted functions as sections of holomorphic line bundles over $P_1(C) \times P_1(C)$. As an example of a nontrivial bundle, we discuss the complex null cone in some detail.

INTRODUCTION

In recent work on general relativity, certain weighted scalars known as "spin and conformally weighted functions" have played a prominent role. During the past few years, in conjunction with work on complex space-time and twistor theory,^{1,2} it has become necessary to consider the "complexifications" of these functions. Our purpose in this paper is to identify these scalars as sections of certain line bundles and to discuss some of their properties from this point of view.

Since the material related to the real two-sphere is already known in another form,³ we shall just review it briefly and concentrate our attention on the holomorphic line bundles which appear in the discussion of complex space-times. Most of the formalism for the real case, developed in Sec. 2, carries over virtually unchanged, although some subtle and important differences do occur. For example, in Sec. 3, we show that the complex null cone is actually a nontrivial C^* -bundle over its space of generators. In Sec. 4, we exhibit complex null infinity as a nontrivial bundle and examine its holomorphic global cross sections; these are the "good cuts" of Newman and his coworkers.^{4,4} Each cut is doubly ruled by the asymptotic twistors of Penrose.² Those asymptotic twistors "not entirely on C' " are shown to be line bundles obtained from complex null infinity by suitable restrictions.

1. PRELIMINARIES

We begin by reviewing two ways of constructing line bundles (i. e., one complex-dimensional vector bundles) over a differentiable manifold M .^{5,6}

The first method involves patching together the trivial bundles $\{U_\alpha \times C\}$ over an open cover $\{U_\alpha\}$ of M . Suppose given, for each nonempty double intersection, a map $h_{\alpha\beta}: U_\alpha \cap U_\beta \rightarrow C^*$, where C^* is the multiplicative group of nonzero complex numbers. Provided that $h_{\alpha\beta}h_{\beta\gamma} = h_{\alpha\gamma}$ in any nonempty triple intersection, we can glue these bundles together in a consistent fashion: If $x \in U_\alpha \cap U_\beta$, then the pair (x, z_β) in $U_\beta \times C$ is identified with $(x, h_{\alpha\beta}(x)z_\beta)$ in $U_\alpha \times C$. The transition functions $\{h_{\alpha\beta}\}$ determine the line bundle completely. A section s of the bundle is given by a set of maps $\{s_\alpha: U_\alpha \rightarrow C\}$ satisfying $s_\alpha = h_{\alpha\beta}s_\beta$ in $U_\alpha \cap U_\beta$; s_α is called the local representative of s in U_α . The bundle is C^∞ provided that each $h_{\alpha\beta}$ is C^∞ ; if M is a complex manifold and each $h_{\alpha\beta}$ is holomorphic, the line bundle is said to be holomorphic.

The second construction begins with a principal bundle $\pi: P \rightarrow M$ with structure group G .⁵ Let ρ be a representation of G on C . Define an equivalence relation on $P \times C$ by $(p, z) \sim (pg, \rho(g^{-1})z)$ for all $g \in G$, and denote the equivalence class of (p, z) by $\{p, z\}$.⁷ The set of all equivalence classes, $B(\rho)$, is a line bundle over M with projection $\pi(\{p, z\}) = \pi(p)$. In terms of the previous construction, it is not difficult to verify that if P is defined by the transition functions $\{r_{\alpha\beta}\}$, then $B(\rho)$ is defined by the transition functions

$$h_{\alpha\beta} = \rho(r_{\alpha\beta}). \quad (1.1)$$

Now suppose we are given a section $s: M \rightarrow B(\rho)$. Let $p \in P$ with $\pi(p) = x$. Denote the component of $s(x)$ in the frame p by $\tilde{s}(p)$:

$$s(\pi(p)) = \{p, \tilde{s}(p)\}. \quad (1.2)$$

This defines a complex-valued function on the principal bundle P . Note that, for $g \in G$, $s(\pi(pg)) = \{pg, \tilde{s}(pg)\} = \{pg, \tilde{s}(pg)\}$, so that

$$\tilde{s}(pg) = \rho(g^{-1})\tilde{s}(p). \quad (1.3)$$

Conversely, any function satisfying (1.3) gives rise to a section of $B(\rho)$; this correspondence is 1-1.

To relate this alternative construction to the first one, let $\{U_\alpha\}$ be an open cover of M such that for each α there exists a local cross section $e_\alpha: U_\alpha \rightarrow P|U_\alpha$. Then each $\{p, z\} \in B(\rho)|U_\alpha$ has a unique representative (e_α, z_α) , and we assign to $\{p, z\}$ the local coordinates $(\pi(e_\alpha), z_\alpha) \in U_\alpha \times C$. In $U_\alpha \cap U_\beta$, we have $e_\alpha = e_\beta r_{\beta\alpha}$, where $r_{\beta\alpha}: U_\beta \cap U_\alpha \rightarrow G$, and the transition functions for $B(\rho)$ are given by (1.1). If s is a section of $B(\rho)$, its local representative in U_α is given simply by

$$s_\alpha = \tilde{s}(e_\alpha). \quad (1.4)$$

We shall use this construction extensively in what follows.

2. SPIN AND CONFORMALLY WEIGHTED FUNCTIONS ON S^2

Consider the principal C^* -bundle $\pi: C^2 - \{0\} \rightarrow P_1(C) \cong S^2$ determined by $\pi: (\xi^0, \xi^1) \rightarrow [\xi^0, \xi^1]$ (homogeneous coordinates). For any complex number w and any integer or half-integer s , the mapping $(s, w): \lambda \rightarrow \lambda^{(s-w)\lambda^{-1} - (s+w)}$ is a representation of C^* on C ; using this, we construct a line bundle $B(s, w) \rightarrow S^2$. By means

of (1.3), a cross section of $B(s, w)$ may be identified with a function $f(\xi^0, \xi^1, \bar{\xi}^0, \bar{\xi}^1) = f(\xi^A, \bar{\xi}^{A'})$ homogeneous of degree $(w - s, w + s)$:

$$f(\lambda \xi^A, \bar{\lambda} \bar{\xi}^{A'}) = \lambda^{w-s} \bar{\lambda}^{w+s} f(\xi^A, \bar{\xi}^{A'}), \quad \lambda \in C^*. \quad (2.1)$$

{Technically [cf. (1.3)], we should write the argument of f as $\xi^A \lambda$; obviously, $\xi^A \lambda = \lambda \xi^A$.}

The sections of $B(s, w)$ are called functions of spin weight s and conformal weight w . To see that this agrees with the usual definition, it is necessary to introduce a particular local trivialization of the principal bundle:

For each $\beta = (\beta^A_B) \in \text{SL}(2, C)$, define a local complex coordinate on S^2 by $\zeta_\beta([\xi^0, \xi^1]) = \xi^0_\beta / \xi^1_\beta$, where $\xi^A_\beta = \beta^A_B \xi^B$. The domain of ζ_β is the open set U_β defined by $\xi^1_\beta \neq 0$. Put $P_\beta = (1 + \zeta_\beta \bar{\zeta}_\beta)^{1/2}$ and define a local cross section $e_\beta: U_\beta \rightarrow C^2 - \{0\} | U_\beta$ by

$$e_\beta = (\xi^0 / \xi^1 P_\beta, \xi^1 / \xi^1 P_\beta). \quad (2.2)$$

If α is another element of $\text{SL}(2, C)$, then clearly

$$e_\alpha = e_\beta (\zeta^1_\beta P_\beta / \zeta^1_\alpha P_\alpha) \text{ in } U_\alpha \cap U_\beta. \quad (2.3)$$

Thus $r_{\alpha\beta} = \zeta^1_\alpha P_\alpha / \zeta^1_\beta P_\beta$; and using (1.1), the transition functions for $B(s, w)$ are given by

$$h_{\alpha\beta} = (r_{\alpha\beta})^{s-w} (\bar{r}_{\alpha\beta})^{-s-w} = \left(\frac{\zeta^1_\alpha / \zeta^1_\beta}{\bar{\zeta}^1_\alpha / \bar{\zeta}^1_\beta} \right)^s \left(\frac{1 + \zeta_\beta \bar{\zeta}_\beta}{|\zeta^0_\alpha / \zeta^1_\alpha|^2 + |\zeta^1_\alpha / \zeta^1_\alpha|^2} \right)^w. \quad (2.4)$$

If we let $\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \alpha \beta^{-1}$, and note that $\zeta_\alpha = (a \zeta_\beta + b) / (c \zeta_\beta + d)$, this becomes

$$h_{\alpha\beta}(\zeta_\beta, \bar{\zeta}_\beta) = \left(\frac{c \zeta_\beta + d}{\bar{c} \bar{\zeta}_\beta + \bar{d}} \right)^s \left(\frac{1 + \zeta_\beta \bar{\zeta}_\beta}{|a \zeta_\beta + b|^2 + |c \zeta_\beta + d|^2} \right)^w. \quad (2.5)$$

Recalling that the local representatives $\{s_\alpha\}$ of a section of $B(s, w)$ satisfy $s_\alpha = h_{\alpha\beta} s_\beta$, we have shown that these are precisely the functions of spin weight s and conformal weight w as defined in Refs. 3, 8.

It should be noted that although these bundles are all different from the standpoint of representation theory,⁹ they are not all topologically distinct. In fact $B(s, w)$ is isomorphic to $B(s, 0)$, for all w . One way to see this is to observe that the defining representations (s, w) and $(s, 0)$ are homotopic to one another (Ref. 5, pp. 27–29), the homotopy being given simply by $\{(s, tw) : t \in [0, 1]\}$. To conclude this section, we recall that any smooth line bundle is completely characterized by its Chern class,⁵ which for S^2 is an element of $H^2(S^2; Z) \cong Z$. Though we do not give the proof here, it is not difficult to show that the Chern class of $B(s, w)$ is given by $-2s \in Z$.

3. HOLOMORPHIC BUNDLES OVER $S^2 \times S^2$

In dealing with complex space–times, one often encounters “complexified” functions of definite spin and conformal weight. Examples include the asymptotic shear of a complex null hypersurface and the related “cut functions” of Newman and co-workers.^{1,4}

Intuitively, one simply proceeds by analytic continua-

tion: If $f(\xi^A, \bar{\xi}^{A'})$ is real analytic, and homogeneous of degree $(w - s, w + s)$ in $(\xi^A, \bar{\xi}^{A'})$, then $f(\xi^A, \eta^{A'})$ is a holomorphic function of four complex variables, defined in an open neighborhood of the “real slice” $\eta^{A'} = \bar{\xi}^{A'}$. By analogy with the real case, one expects these functions to correspond to sections of certain holomorphic line bundles over the “complexification” of S^2 . We shall see below that this implies a restriction on the possible values of s and w .

To proceed rigorously, we consider the principal $C^* \times C^*$ bundle $\pi: (C^2 - \{0\}) \times (C^2 - \{0\}) \rightarrow P_1(C) \times P_1(C) \cong S^2 \times S^2$; the mapping π sends the pair $(\xi^A, \eta^{A'})$ to $([\xi^A], [\eta^{A'}])$. The base space should be regarded as the projective space of complex null directions at some fixed point in a complex space–time. We denote the total space of the bundle by E .

Notice that the points $([\xi^A], [\eta^{A'}])$ of $P_1(C) \times P_1(C)$ are in one-to-one correspondence with the proportionality classes of nonzero, singular 2×2 matrices $[\xi^A \eta^{A'}]$. We shall use this identification in the following.

The only holomorphic representations of $C^* \times C^*$ on C are given by $(\lambda, \mu) \rightarrow \lambda^m \mu^n$, where m and n are integers. We set $s = (m - n)/2$, $w = -(m + n)/2$; note that w and s are either both integer or half-integer depending on whether m and n have the same or opposite parity. Sections of the resulting bundles $\tilde{B}(s, w)$ are in one-to-one correspondence with holomorphic functions on E satisfying

$$f(\lambda \xi^A, \mu \eta^{A'}) = \lambda^{w-s} \mu^{w+s} f(\xi^A, \eta^{A'}). \quad (3.1)$$

By restricting $\tilde{B}(s, w) \rightarrow P_1(C) \times P_1(C)$ to each of the factors of the base, one easily shows that the Chern class of this bundle is given by $(w - s, w + s) \in H^2(P_1 \times P_1, Z) \cong Z \times Z$. Thus, if $(s, w) \neq (s', w')$, the bundles $\tilde{B}(s, w)$ and $\tilde{B}(s', w')$ are topologically, and hence analytically, inequivalent, a significant difference from the situation in the real case. Note, in particular, that none of these bundles is a product except for $\tilde{B}(0, 0)$.

Example: The complex null cone

In a real space–time, the nonzero null vectors at any given point form a trivial R^* -bundle over the 2-sphere of real null directions; in a complex space–time, however, the analogous bundle is nontrivial. To see this, choose and fix a spin frame at the point in question, so that any nonzero null vector may be represented in the form $\xi^A \eta^{A'} \neq 0$. Of course, the same vector may be written as $\pi^A \tau^{A'}$, where $\pi^A = \alpha \xi^A$ and $\tau^{A'} = \alpha^{-1} \eta^{A'}$, for any $\alpha \in C^*$. The mapping $\xi^A \eta^{A'} \rightarrow [\xi^A \eta^{A'}]$ exhibits the complex null cone CN as a C^* -bundle over $P_1(C) \times P_1(C)$.

Now consider the C^* -bundle obtained from $\tilde{B}(0, 1)$ by deleting the zero section. Recall that an element of this bundle is an equivalence class $\{(\xi^A, \eta^{A'}), z\}$, with $z \in C^*$ and $\{(\xi^A, \eta^{A'}), z\} \sim \{(\lambda \xi^A, \mu \eta^{A'}), \lambda \mu z\}$ for $(\lambda, \mu) \in C^* \times C^*$. It is clear that the mapping $\{(\xi^A, \eta^{A'}), z\} \rightarrow z^{-1} \xi^A \eta^{A'}$ is a holomorphic bundle isomorphism of $\tilde{B}(0, 1) - \{\text{zero section}\}$ onto CN . Thus the complex null cone is a nontrivial C^* -bundle over its space of generators. This means in particular that, in contrast to

the real case, the complex null cone has no global cross-sections or "cuts."¹² This situation may be remedied by adding back the zero section in an appropriate way, as we shall see below.

4. THE STRUCTURE OF COMPLEX NULL INFINITY

The conformal compactification of complex Minkowski space is obtained as follows (see Ref. 13 for the analogous construction in the real case):

Define a complex metric on C^6 by $h(y, y) = (y^0)^2 - (y^1)^2 - \dots - (y^4)^2 + (y^5)^2$, and let \mathcal{N} be the set of all nonzero null vectors. If $y \in \mathcal{N}$, so is λy for all $\lambda \in C^*$, and the conformal compactification $C\mathcal{M} = \mathcal{N}/C^*$ is a well-defined compact complex 4-manifold in $P_5(C)$. The space $C\mathcal{M}$ is well known to mathematicians as the Grassmann manifold of lines in $P_3(C)$. Denote the image of y in $C\mathcal{M}$ by its homogeneous coordinates $[y^a]$.

Complex Minkowski space, CM^4 , is naturally embedded in $C\mathcal{M}$, via

$$\phi(z^\mu) = [z^\mu, \frac{1}{2}(1 + z \cdot z), \frac{1}{2}(1 - z \cdot z)], \quad z \cdot z = z^\nu z_\nu. \quad (4.1)$$

It is easily checked that the image of ϕ contains all points of $C\mathcal{M}$ except those for which $y^4 + y^5 = 0$. These exceptional points have the form $[y^\mu, y^4, -y^4]$, where $y^\mu y_\mu = 0$ and not all $y^a = 0$. The complex 3-manifold obtained from them by deleting the singular point $I = [0, +1, -1]$ is called complex null infinity and denoted by $C\mathcal{J}$. Precisely as in the real case any null geodesic $\{z^\mu + \lambda b^\mu : \lambda \in C, b \cdot b = 0\}$ in CM^4 has a unique "end point" on $C\mathcal{J}$ given by

$$\lim_{\lambda \rightarrow \infty} [\phi(z^\mu + \lambda b^\mu)] = [b^\mu, z \cdot b, -z \cdot b]. \quad (4.2)$$

Changing to spinor coordinates and putting $\xi = y^4 = -y^5$, $C\mathcal{J}$ may be represented by the submanifold of $P_4(C)$ given by

$$C\mathcal{J} = \{[\xi^A \eta^{A'}, \xi] : \xi^A \eta^{A'} \neq 0, \xi \in C\}, \quad (4.3)$$

which exhibits $C\mathcal{J}$ as a line bundle over $P_1(C) \times P_1(C)$. The projection is given simply by $\pi : [\xi^A \eta^{A'}, \xi] \rightarrow [\xi^A \eta^{A'}]$ and the vector space structure is defined as follows: If $\pi([\xi^A \eta^{A'}, z]) = \pi([\sigma^A \tau^{A'}, w])$, there is a unique $\lambda \in C^*$ such that $\lambda \sigma^A \tau^{A'} = \xi^A \eta^{A'}$; we set

$$[\sigma^A \tau^{A'}, w] + [\xi^A \eta^{A'}, \xi] := [\xi^A \eta^{A'}, \lambda w + \xi]. \quad (4.4)$$

We may now observe that the mapping $\{(\xi^A, \eta^{A'}), \xi\} \rightarrow [\xi^A \eta^{A'}, \xi]$ defines a vector bundle isomorphism between $\tilde{B}(0, 1)$ and $C\mathcal{J}$. Thus, the difference between $C\mathcal{N}$ and $C\mathcal{J}$ is just the difference between a C^* -bundle and the naturally associated line bundle.

Using (4.2), we see that the zero section of $C\mathcal{J}$ is just the set of "end points" of all null geodesics passing through the point 0 in CM^4 . From the standpoint of I , of course, it is the null cone at 0 which is "at infinity", so that $C\mathcal{J}$ minus its zero section is just the (ordinary) complex null cone of the point I .

In contrast to $C\mathcal{N}$, $C\mathcal{J}$ admits a four-dimensional vector space of global sections; these are precisely the "good cuts." If $z^{AA'}$ is an arbitrary point of CM^4 , and $z^{AA'}$ is an arbitrary point of CM^4 , and $z^{AA'} + \lambda \xi^A \eta^{A'}$ is a null geodesic through $z^{AA'}$, it intersects $C\mathcal{J}$ in the point $[\xi^A \eta^{A'}, z_{AA'} \xi^A \eta^{A'}]$ [see (4.2)]. Notice that this point depends only on the direction $([\xi^A], [\eta^{A'}])$ of the geodesic through $z^{AA'}$. As the direction varies, we obtain the global cross section

$$Z : [\xi^A \eta^{A'}] \rightarrow [\xi^A \eta^{A'}, z_{AA'} \xi^A \eta^{A'}] \quad (4.5)$$

of $C\mathcal{J}$. The section Z can be concisely represented as a holomorphic function on E :

$$Z(\xi^A, \eta^{A'}) = z_{AA'} \xi^A \eta^{A'}. \quad (4.6)$$

Conversely, any section of C defines a holomorphic function homogeneous of degree (1, 1) on $E = C^2 - \{0\}$; since any such function is automatically an entire function (Hartog's theorem, Ref. 14, pp. 50ff.), it must be a polynomial such as that in (4.6). Thus the sections of $C\mathcal{J}$ are parametrized by the points of CM^4 , and form a four-dimensional vector space, as asserted. In any trivialization of $C\mathcal{J}$, the local representatives $u_\alpha = Z(\xi_\alpha, \eta_\alpha)$ of Z will be characterized as solutions to the differential equation

$$\delta_\alpha^2 Z = 0. \quad (4.7)$$

We conclude with a few remarks concerning asymptotic twisters. At any point $z^{AA'}$ of CM^4 , the null cone is generated by totally null two-planes (twistor surfaces⁴) of the form

$$\{z^{AA'} + \xi^A \eta_0^{A'} : \eta_0^{A'} \text{ fixed } \neq 0, \xi^A \neq 0\}. \quad (4.8)$$

This surface intersects $C\mathcal{J}$ in the set $\{[\xi^A \eta_0^{A'}, z_{AA'} \xi^A \eta_0^{A'}]\}$, a projective asymptotic twistor of CM^4 .² Clearly, each section of $C\mathcal{J}$ is ruled by asymptotic twisters. Of course, $C\mathcal{J}$ itself is also generated by twistor surfaces. These have the form (in the valence $[\frac{1}{0}]$ case) $\{[\xi^A \eta^{A'}, z] : z \in C, \xi^A \text{ fixed } \neq 0, \eta^{A'} \neq 0\}$, and are actually line bundles over $P_1(C)$. They correspond to the restriction of $C\mathcal{J} \rightarrow P_1(C) \times P_1(C)$ to $\{[\xi^A]\} \times P_1(C)$. Similar remarks apply to the valence $[\frac{1}{1}]$ asymptotic twisters.

¹E. T. Newman, *Gen. Rel. Grav.* **7**, 107 (1976).

²R. Penrose, article in *Quantum Gravity*, edited by C. Isham *et al.* (Oxford U. P., London, 1975).

³A. Held, E. T. Newman, and R. Posadas, *J. Math. Phys.* **11**, 3145 (1970).

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⁵D. Husemoller, *Fiber Bundles* (McGraw-Hill, New York, 1966).

⁶S. Kobayashi and K. Nomizu, *Foundations of Differential Geometry, I, II* (Wiley, New York, 1963, 1969).

⁷ $\{p, z\}$ is a vector at $\pi(p)$. z is its "component" in the "frame" p , while $\rho(g^{-1})z$ is its component in the frame pg .

⁸E. T. Newman and R. Penrose, *J. Math. Phys.* **7**, 863 (1966).

⁹See either Ref. 10 or Ref. 11. The space $C^2 - \{0\}$ is the homogeneous space $SL(2, C)/T^2$, where T^2 is the Abelian group

$$\left\{ \begin{bmatrix} 1 & z \\ 0 & 1 \end{bmatrix} \right\} : z \in C;$$

the sphere is the homogeneous space $SL(2, C)/C^* \circ T^2$. If we induce with the representation $(s, w) : (\lambda, z) \rightarrow \lambda^{s+w} \bar{\lambda}^{-(s+w)}$, the resulting C -valued functions on $SL(2, C)$ are constant on the cosets of T^2 ; i. e., they are functions on $C^2 - \{0\}$. This is the group-theoretical origin of the bundles $B(s, w)$.

¹⁰I. M. Gel'fand, *et al.*, *Generalized Functions*, Vol. 5 (Academic, New York, 1966).

¹¹N. Wallach, *Harmonic Analysis on Homogeneous Spaces* (Dekker, New York, 1973).

¹²A *principal* bundle is trivial \Leftrightarrow it admits a global cross section. Any global cross section of $\tilde{B}(0, 1) - \{\text{zero section}\}$ gives rise to a cross section of $\tilde{B}(0, 1)$ itself; but as we shall see in the next section, any cross section of $\tilde{B}(0, 1)$ is represented by a polynomial and therefore has zeroes. Thus the principle bundle has no global cross section.

¹³D. Lerner, *J. Math. Phys.* 18, 1812 (1977).

¹⁴R. Narasimhan, *Several Complex Variables* (University of Chicago Press, Chicago, 1971).

Wavefunctions of identical particles

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We present a description of the quantum mechanical states of a system of n indistinguishable particles moving on a manifold M by \mathbb{C}/S_2 -valued functions ψ' defined on the configuration space M^n/S_n . These functions satisfy one of two homotopy conditions, which characterize the particles as bosons or fermions. Any closed curve of M^n/S_n which does not intersect the diagonals can be classified as even or odd according to whether its lifts to M^n have end points in M^n which are even or odd permutations of each other. For bosons, ψ' must map any such closed curve which also avoids $\ker\psi'$ onto an even number of basic loops of $(\mathbb{C}-\{0\})/S_2$. For fermions, ψ' must map such even loops of M^n/S_n onto an even number, and odd loops onto an odd number, of basic loops of $(\mathbb{C}-\{0\})/S_2$.

1. INTRODUCTION

A system of n distinguishable particles all moving on a manifold M has for its configuration space the Cartesian product $M^n = M \times \dots \times M$ (n times). Elements of M^n are ordered n -tuples (m_1, \dots, m_n) of points of M . If the particles are indistinguishable all permutations of (m_1, \dots, m_n) describe the same configuration. The configuration is now the *unordered set* of points $\{m_1, \dots, m_n\}$. The configuration space is the quotient space M^n/S_n , where the permutation group S_n acts on M^n by permuting the n -tuples. Observables correspond to functions on the cotangent bundle $T^*(M^n/S_n)$. This point has been made earlier.^{1,2}

In quantum mechanics, if the particles are bosons, their state is conventionally described by a fully symmetric complex valued wavefunction ψ defined on M^n . Such a function can equally well be regarded as defined on M^n/S_n . Symmetric functions on M^n are in one-to-one correspondence with functions on M^n/S_n .

If the particles are fermions however, the conventional description of the state is by a fully antisymmetric complex function ψ on M^n ; that is, not by any function on the configuration space but by a function on a covering space. The order of the arguments of ψ is physically irrelevant but is required mathematically, since an odd permutation of this order alters the sign of ψ . The conventional mathematical description is thus slightly redundant. This makes it desirable to see whether one can formulate a description of the states of n fermions using functions defined on the physically significant configuration space M^n/S_n rather than by functions on M^n satisfying auxiliary symmetry conditions. Unfortunately however, an antisymmetric function $\psi : M^n \rightarrow \mathbb{C}$ does not in general determine a complex valued function ψ' (even modulo an overall sign) on the quotient space M^n/S_n , but only a mapping from M^n/S_n to \mathbb{C}/S_2 , where the nontrivial element of S_2 acts on \mathbb{C} by changing the sign. If $\dim M > 1$, one can usually join the points $(m_1, m_2, m_3, \dots, m_n)$ and $(m_2, m_1, m_3, \dots, m_n)$ of M^n by a curve γ on which ψ never vanishes; the values of ψ at the end points of γ are equal except for sign. Now the projection of this curve γ onto M^n/S_n is a *closed loop* $p\gamma$. If we choose say

$$\psi'(\{m_1, \dots, m_n\}) = +\psi(m_1, m_2, m_3, \dots, m_n)$$

and fix ψ' on the loop $p\gamma$ by continuity, then on complet-

ing the loop we obtain a contradiction in sign at $\{m_1, \dots, m_n\}$. (In the case $M = \mathbb{R}$, the curve γ must intersect the diagonal, where $\psi = 0$. An antisymmetric function $\psi : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{C}$ does indeed determine a complex function ψ' on the half-space $(\mathbb{R} \times \mathbb{R})/S_2$ up to an overall sign. The case when M is a circle is an interesting exercise.)

Thus if we wish to describe the state of a system of n identical fermions by means of a function on its configuration space M^n/S_n , we are forced into using \mathbb{C}/S_2 valued functions. In the next section we derive homotopy criteria which are necessary and sufficient for a mapping

$$\psi' : M^n/S_n \rightarrow \mathbb{C}/S_2$$

to determine by lifting (modulo an overall sign) a symmetric or an antisymmetric mapping $\psi : M^n \rightarrow \mathbb{C}$. The homotopy theory involved is quite straightforward and is well explained in the first twenty five pages of Greenberg's book.³ The mathematical literature on the topology of configuration spaces may be traced from the paper by McDuff.⁴

2. THE HOMOTOPY CRITERIA

We need two results from the elementary homotopy theory of covering spaces, which may be found in Chaps. 5 and 6 of Greenberg's book.

(I) Let E be a pathwise connected topological space and let G be a group of homeomorphisms of E which operates properly discontinuously (any $e \in E$ has a neighborhood V such that $V \cap gV = \emptyset$ for all $g \neq 1$ in G). Let $p : E \rightarrow E/G$ be the projection onto the orbit space. Then the sequence

$$1 \rightarrow \pi_1(E) \xrightarrow{p_*} \pi_1(E/G) \rightarrow G \rightarrow 1$$

is exact, i. e., G is isomorphic to the quotient group $\pi_1(E/G)/p_*\pi_1(E)$ of the fundamental groups.

(II) Let $(e_0, E), (x_0, X), (y_0, Y)$ be pathwise connected pointed topological spaces. Let $\psi' : (y_0, Y) \rightarrow (x_0, X)$ be any map and let $q : (e_0, E) \rightarrow (x_0, X)$ be a covering space map. Then there is a (unique) lifting $\psi : (y_0, Y) \rightarrow (e_0, E)$ of ψ' , ($q\psi = \psi'$) if and only if $\psi'_*\pi_1(y_0, Y) \subset q_*\pi_1(e_0, E)$.

We should like to apply these results to our situation which may be drawn as follows:

$$\begin{array}{ccc}
M^n & \xrightarrow{p} & M^n/S_n \\
\psi \downarrow & & \downarrow \psi' \\
\mathbb{C} & \xrightarrow{q} & \mathbb{C}/S_2
\end{array}$$

where we are given ψ' and wish to construct ψ . M is assumed to be pathwise connected. However, neither p nor q is a covering space map, because p is not a homeomorphism of neighborhoods of diagonal elements in M^n and q is not a homeomorphism of neighborhoods of zero in \mathbb{C} . Another way to put it is to say that S_1 and S_2 do not act properly discontinuously on M^n and \mathbb{C} respectively. However, if D is the set of all diagonal elements of M^n ,

$$D = \{(m_1, \dots, m_n) : m_i = m_j \text{ for some } i \neq j\}$$

then S_n acts properly discontinuously on $M^n \setminus D$. Further, S_2 acts properly discontinuously on $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$.

Let $K(\psi') \subset M^n$ be the kernel of the map $\psi' \circ p$, and denote $\mathcal{M} = M^n \setminus (D \cup K(\psi'))$. We shall suppose \mathcal{M} is still pathwise connected. (If it were not, we should consider each component separately.) Then S_n acts properly discontinuously on \mathcal{M} , and we consider the problem of constructing ψ in the diagram of maps between pointed sets,

$$\begin{array}{ccc}
(\tilde{\alpha}, \mathcal{M}) & \xrightarrow{p} & (\alpha, \mathcal{M}/S_n) \\
\psi \downarrow & \dashrightarrow & \downarrow \psi' \\
(\tilde{z}, \mathbb{C}^*) & \xrightarrow{q} & (z, \mathbb{C}^*/S_2)
\end{array}$$

so that the diagram commutes.

The corresponding diagram of fundamental groups is

$$\begin{array}{ccccc}
1 & \rightarrow & \pi_1(\mathcal{M}) & \xrightarrow{p_*} & \pi_1(\mathcal{M}/S_n) & \xrightarrow{\nu} & S_n & \rightarrow & 1 \\
& & \downarrow \psi'_* & & \downarrow \mu & & & & \\
1 & \rightarrow & \pi_1(\mathbb{C}^*) & \xrightarrow{q_*} & \pi_1(\mathbb{C}^*/S_2) & \xrightarrow{\lambda} & S_2 & \rightarrow & 1.
\end{array}$$

Here, by (I), the rows are exact. The map $\mu : S_n \rightarrow S_2$ is the parity map whose kernel is the group of even permutations. We do not claim that $\mu \circ \nu = \lambda \circ \psi'_*$. The point $\tilde{\alpha}$ is chosen arbitrarily in \mathcal{M} , and determines the points α and z . The point \tilde{z} may be chosen to be either of the two points sitting over z (and in the fermion case will turn out to fix the sign of the wavefunction ψ). In the lower row, $\pi_1(\mathbb{C}^*) = \mathbb{Z}$ and $q_* \pi_1(\mathbb{C}^*) = 2\mathbb{Z} \subset \pi_1(\mathbb{C}^*/S_2) = \mathbb{Z}$. Thus q_* simply multiplies by 2, to produce the normal subgroup of even elements of $\pi_1(\mathbb{C}^*/S_2)$, which in turn gets mapped to zero by λ . The odd elements of $\pi_1(\mathbb{C}^*/S_2)$ get mapped to the nontrivial element of S_2 .

It follows from the lifting criterion (II) that the map ψ exists such that $q \circ \psi = \psi' \circ p$ iff $(\psi' \circ p)_* \pi_1(\mathcal{M}) \subset q_* \pi_1(\mathbb{C}^*)$, i. e., iff $\lambda \circ \psi'_* \circ p_* = 0$, i. e., iff $\psi' \circ p$ maps all loops in \mathcal{M} to even loops in \mathbb{C}^*/S_2 . For such a ψ' there are two cases to consider.

(i) Bose. If $\lambda \circ \psi'_* = 0$, i. e., iff ψ' maps all loops in \mathcal{M}/S_n to even loops in \mathbb{C}^*/S_2 , then ψ' itself lifts to a map $\tilde{\psi} : (\alpha, \mathcal{M}/S_n) \rightarrow (\tilde{z}, \mathbb{C}^*)$, and the map $\psi = \tilde{\psi} \circ p$ is a fully symmetric complex valued function defined on \mathcal{M} . We may extend ψ to the whole of M^n by continuity. (Note that in this case $\lambda \circ \psi'_* = 0$ but $\mu \circ \nu \neq 0$ so the diagram of fundamental groups does not commute in the right-hand square.)

(ii) Fermi. If $\lambda \circ \psi'_* \circ p_* = 0$ but $\lambda \circ \psi'_* \neq 0$, then $\lambda \circ \psi'_*$ must map onto S_2 . Then no map $\tilde{\psi} : \mathcal{M}/S_n \rightarrow \mathbb{C}^*$ exists that $q \circ \tilde{\psi} = \psi'$, but there still exists a map $\psi : \mathcal{M} \rightarrow \mathbb{C}^*$ such that $q \circ \psi = \psi' \circ p$. We seek the further condition on ψ' that ψ should be antisymmetric.

Consider a closed loop l in \mathcal{M}/S_n through α . It has a unique lift $\tilde{l} = p^{-1}l$ through $\tilde{\alpha}$ in \mathcal{M} , which will be a (generally open) curve joining $\tilde{\alpha}$ to a point $\tilde{\beta}$ with $p(\tilde{\alpha}) = p(\tilde{\beta}) = \alpha$. Writing $\tilde{\alpha} = (\alpha_1, \dots, \alpha_n)$, $\tilde{\beta} = (\beta_1, \dots, \beta_n)$ we have that $\alpha_j = \beta_{s_j}$, where $s : (1, \dots, n) \rightarrow (s_1, \dots, s_n)$ is the element of the permutation group S_n which labels the coset in $\pi_1(\mathcal{M}/S_n)$ containing the homotopy class $[l]$ of l ,

$$s = \nu([l]).$$

It is convenient now to use multiplication as the group operation in S_2 and to label the elements of S_2 as $\epsilon = \pm 1$. Let $\mu \circ \nu([l]) = \epsilon$. Then the permutation $s : \tilde{\alpha} \mapsto \tilde{\beta}$ has parity ϵ and if ψ is antisymmetric then $\psi(\tilde{\beta}) = \epsilon \psi(\tilde{\alpha})$. So $\psi(\tilde{l})$ is an open or closed curve in \mathbb{C}^* depending on whether $\epsilon = -1$ or $\epsilon = +1$, and correspondingly $[q\psi\tilde{l}]$ is odd or even, i. e., $\lambda[q\psi\tilde{l}] = \epsilon$. Thus

$$\lambda[q\psi\tilde{l}] = \mu \circ \nu([l]) = \mu \circ \nu([p\tilde{l}]).$$

But $q \circ \psi = \psi' \circ p$, so

$$\lambda[\psi'p(\tilde{l})] = \mu \circ \nu[p(\tilde{l})],$$

i. e.,

$$\lambda \circ \psi'_*[l] = \mu \circ \nu[l].$$

Hence a necessary (and evidently sufficient) condition for there to exist an antisymmetric lift ψ of ψ' is that $\lambda \circ \psi'_* = \mu \circ \nu$, i. e., that the right-hand square commutes in the diagram of fundamental groups.

We conclude with some remarks about the principle of superposition of states. This requires that pure states be in (1, 1) correspondence with one-dimensional subspaces (rays) of a Hilbert space. The functions $\psi' : M^n/S_n \rightarrow \mathbb{C}/S_2$ which satisfy the Bose (Fermi) homotopy condition do not form a linear space, since \mathbb{C}/S_2 is not a linear space. What we have shown above is that each of these functions ψ' determines a ray in the Hilbert space \mathcal{H}_S (\mathcal{H}_A) of symmetric (antisymmetric) complex-valued functions on the covering space M^n . Two functions ψ' differing by a constant phase factor determine the same ray. Thus we have established a (1, 1) correspondence between the rays of \mathcal{H}_S (\mathcal{H}_A) and the equivalence classes of \mathbb{C}/S_2 -valued functions ψ' modulo overall phase defined on the configuration space M^n/S_n which satisfy the Bose (Fermi) homotopy condition.

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Geometry of motion of a single elastic body point

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A four-dimensional space $L^{\hat{X}}$, in which body point \hat{X} of a simple elastic body describes a geodesic line during the process of deformation, is constructed. It is shown that $L^{\hat{X}}$ is a torsion-free non-Riemannian space. The structure of $L^{\hat{X}}$ is examined for universal dynamical solutions for incompressible elastic bodies.

1. INTRODUCTION

Use of the concepts of differential geometry in classical mechanics has theoretical as well as pragmatic value. On one hand the results obtained from the geometrical considerations give deep insight into the motion of the system by revealing some of the intrinsic properties that the trajectory of the system has, while on the other hand they could be used for the solution of concrete problems. Stability analysis¹ based on the Synge's theory of perturbances² is just one example of the practical use, in mechanics, of the results obtained by the differential geometry methods.

The aim of this paper is to study motion of a single elastic body point along the lines of Refs. 3–5. Motion of an elastic body point⁶ can be analyzed in four-dimensional (three spatial coordinates and time) space E_4 called Newtonian space–time. To each body point \hat{X} there corresponds a smooth curve $l^{\hat{X}}$ in E_4 , called world line, such that during the process of deformation a point in E_4 that corresponds to X “moves” along $l^{\hat{X}}$. Our objective is to construct a four-dimensional space $L^{\hat{X}}$, such that the curve in $L^{\hat{X}}$ that the point \hat{X} describes during the process of deformation is a geodesic line. The problem of finding $L^{\hat{X}}$ with the properties just stated is what is usually called geometrization of motion.

In Sec. 2 we will determine connection coefficients of the space $L^{\hat{X}}$ and discuss some of the properties of the present approach to the motion of an elastic body point, while in Sec. 3 the structure of $L^{\hat{X}}$ will be examined for a class of motions called universal dynamical solutions for incompressible elastic bodies.

2. GEOMETRY OF MOTION OF A SINGLE BODY POINT

Suppose H_0 is the initial configuration of a simple elastic body β . We denote by d_α basis vectors of the coordinate system in H_0 , by $\{\overset{\alpha}{\Gamma}_{\alpha\beta}\}$ Christoffel symbols based on the metric tensor $\hat{g}_{\alpha\beta} = d_\alpha \cdot d_\beta$, and by X^α coordinates of a body point \hat{X} in the configuration H_0 . By H we denote configuration of β at the time instant t , by e_k basis vectors of the coordinate system in H by $\{\overset{k}{\Gamma}_{kl}\}$ Christoffel symbols based on the metric $g_{kl} = e_k \cdot e_l$, and by x^k coordinates of a body point \hat{X} in H . Equations of motion could be written⁷

$$A_k^{(\alpha\beta)} x^m_{,\alpha;\beta} + q_k + \rho_R b_k = \rho_R a_k, \quad (2.1)$$

where q_k is the density of the resultant force due to inhomogeneity per unit volume in H_0 , and is given via constitutive equation H_k^α for the Piola–Kirchhoff stress

tensor as

$$q_k = \frac{\partial H_k^\alpha}{\partial X^\alpha} \quad (2.2)$$

and

$$A_k^{(\alpha\beta)} = \frac{1}{2} [A_k^{\alpha\beta} + A_k^{\beta\alpha}], \quad (2.3)$$

where

$$A_k^{\alpha\beta} = \frac{\partial H_k^\alpha}{\partial F^m_\beta}, \quad (2.4)$$

$F^m_\beta = x^m, \beta = \partial x^m / \partial X^\beta$. Also, in (2.1) ρ_R represents the density of β in H_0 ,

$$x^m_{,\alpha;\beta} = \frac{\partial^2 x^m}{\partial X^\alpha \partial X^\beta} + \left\{ \begin{matrix} m \\ s \ r \end{matrix} \right\} x^s_{,\alpha} x^r_{,\beta} - \left\{ \begin{matrix} \sigma \\ \alpha \ \beta \end{matrix} \right\} x^m_{,\sigma} \quad (2.5)$$

is the total covariant derivative of $x^m_{,\alpha}$ and

$$a^k = \frac{d^2}{dt^2} x^k(X^\alpha, t) + \left\{ \begin{matrix} k \\ s \ r \end{matrix} \right\} \frac{dx^s}{dt} \frac{dx^r}{dt} \quad (2.6)$$

is acceleration of the particle \hat{X} . Denoting by R^k the vector

$$R^k = [A_k^{(\alpha\beta)} x^m_{,\alpha;\beta} + q^k] \frac{1}{\rho_R} + b^k, \quad (2.7)$$

Eq. (2.1) can be written as

$$\frac{d^2}{dt^2} x^k(X^\alpha, t) + \left\{ \begin{matrix} k \\ s \ r \end{matrix} \right\} \frac{dx^s}{dt} \frac{dx^r}{dt} = R^k, \quad X^\alpha \in H_0, t \geq 0. \quad (2.8)$$

In (2.8) R^k is a function of X^α, F^m_β , and t .

In four-dimensional space $L^{\hat{X}}$, we wish to construct an equation of the geodesic line which must be identical to (2.8) for a fixed particle, i.e., fixed X^α . To characterize $L^{\hat{X}}$ we first define its metric \bar{g}_{kr} , $k, r = 1, 2, 3, 4$. In analogy with the geometrization of motion of rheonomic systems of classical mechanics^{3,4} we take

$$\bar{g}_{ml} = g_{ml}, \quad m, l = 1, 2, 3, \\ \bar{g}_{44} = 1, \quad \bar{g}_{4m} = \bar{g}_{m4} = 0, \quad m = 1, 2, 3, 4. \quad (2.9)$$

Denoting by \bar{x}^m , $m = 1, 2, 3, 4$ the coordinates of a point in $L^{\hat{X}}$, differential equations of a geodesic line are

$$\frac{d^2 \bar{x}^m}{ds^2} + \bar{\Gamma}^m_{kl} \frac{d\bar{x}^k}{ds} \frac{d\bar{x}^l}{ds} = 0, \quad m, l, k = 1, 2, 3, 4, \quad (2.10)$$

where s is a parameter and $\bar{\Gamma}^m_{kl}$ are connection coefficients, to be determined. Equations (2.10) must be identical to the equations (2.8) which with $x^1 = \bar{x}^1$,

$x^2 = \bar{x}^2$, $x^3 = \bar{x}^3$, $t = \bar{x}^4$ become

$$\frac{d^2}{d(\bar{x}^4)^2} \bar{x}^m + \left\{ \begin{matrix} k \\ s \end{matrix} \right\} \frac{d\bar{x}^s}{d\bar{x}^4} \frac{d\bar{x}^r}{d\bar{x}^4} = R^k, \quad k, s, r = 1, 2, 3. \quad (2.11)$$

Following^{4,5} we set

$$\bar{\Gamma}_{rk}^m = \left\{ \begin{matrix} m \\ r \ k \end{matrix} \right\} - \frac{1}{\sum_{n=1}^3 (d\bar{x}^n/ds)(d\bar{x}_n/ds)} \bar{g}_{rk} R^m, \quad m, r, k = 1, 2, 3$$

$$R^4 = \bar{\Gamma}_{4k}^r = \bar{\Gamma}_{k4}^r = 0, \quad r, k = 1, 2, 3, 4. \quad (2.12)$$

Then we have:

Theorem: During the process of deformation, body point \hat{X} of a simple elastic body β describes in four-dimensional space $L^{\hat{X}}$ with the metric tensor (2.9) and connection coefficients (2.12) a geodesic line.

Proof: Putting $m = 4$ in (2.10) and using (2.12)₂ we get

$$\frac{d^2 \bar{x}^4}{ds^2} = 0 \quad (2.13)$$

so that $\bar{x}^4 = a \cdot s + b$, $a = \text{const}$, $b = \text{const}$. Choose $a = 1$, $b = 0$. Then, Eq. (2.10) becomes

$$\frac{d^2 \bar{x}^m}{d(\bar{x}^4)^2} + \bar{\Gamma}_{rk}^m \frac{d\bar{x}^r}{d\bar{x}^4} \frac{d\bar{x}^k}{d\bar{x}^4} = 0, \quad m, r, k = 1, 2, 3. \quad (2.14)$$

Direct substitution of (2.12)₁ into (2.14) gives (2.11) and hence proves the theorem.

In using the theorem just stated to construct space $L^{\hat{X}}$ we will distinguish two special cases that correspond to two special problems of the elasticity theory.

Case 1. The stress field $H_k^\alpha(X^\beta, t)$ is a prescribed function of the coordinates X^α and time t , and we want to find the motion $x^k(X^\alpha, t)$ of a fixed particle \hat{X} . Then, the first two terms on the left-hand side of Eq. (2.1) are known function of X^α and t (since they represent the divergence of the known tensor field H_k^α). Therefore the vector R^k defined by Eq. (2.8) becomes a known function of t for fixed X^α (i.e., fixed particle \hat{X}). In this case the connection coefficients (2.12) are functions of x^k ($k = 1, 2, 3, 4$ and dx^k/ds ($k = 1, 2, 3$)) only. The space with such connections belongs to the class of generalized affine geodesic spaces of Yano.⁸

Case 2. Stress field $H_k^\alpha(X^\beta, t)$ is not known in advance and must be determined together with the motion $x^k(X^\alpha, t)$. In this case the vector R^k is a function of x^k ($k = 1, 2, 3, 4$), dx^k/ds ($k = 1, 2, 3$), F^m_α , and $F^m_{\alpha;\beta}$. For fixed X^α , F^m_α and $F^m_{\alpha;\beta}$ remain unknown functions in the expressions for the connection coefficients. They represent the influence of the motion of the neighboring particles on the path of \hat{X} . Thus Eqs. (2.9) and (2.12) define a family of spaces. In such a case we can not talk about a geodesic line, in its usual meaning. The geometry becomes fixed and $L^{\hat{X}}$ becomes the generalized affine geodesic space of Yano in the case when $F^m_{\alpha;\beta} = 0$, so that R^k again depends on \bar{x}^k ($k = 1, 2, 3, 4$) and $d\bar{x}^k/ds$ ($k = 1, 2, 3$) only.

The connection coefficients (2.12) are singular for the points where \hat{X} is in the state of instantaneous rest,

i.e., where

$$\sum_{m=1}^3 \frac{d\bar{x}^m}{d\bar{x}^4} \frac{d\bar{x}_m}{d\bar{x}^4} = \sum_{m=1}^3 \frac{d\bar{x}^m}{dt} \frac{d\bar{x}_m}{dt} = 0. \quad (2.15)$$

Such singularity of the connection coefficients occurs in other types of geometrization of motion too. (For example in Ref. 9, p. 139 it occurs in the context of Riemannian geometry.) We exclude points where (2.15) holds from analysis.

For fixed X^α Eqs. (2.8) have the same form as the equations of motion of nonconservative dynamical systems, R^k being the nonconservative force. A geometrization of such systems, under the assumption that R^k is a function of generalized coordinates only, is given in Ref. 5. Thus our results could be interpreted, in the context of classical particle mechanics, as geometrization of motion of nonconservative dynamical systems with nonconservative forces dependent on time and generalized coordinates.

From (2.12) we find that

$$\bar{\Gamma}_{rk}^m = \bar{\Gamma}_{kr}^m, \quad (2.16)$$

so that $L^{\hat{X}}$ is torsion free space. To examine its metrical properties we compute the covariant derivative of the metric tensor \bar{g}_{km} with respect to the connection coefficients (2.12). The result is

$$\nabla_m \bar{g}_{ik} = \left(\sum_{n=1}^3 \frac{dx^n}{ds} \frac{dx_n}{ds} \right)^{-1} [\bar{g}_{im} R_k + \bar{g}_{km} R_i]. \quad (2.17)$$

Therefore, the space $L^{\hat{X}}$ is not a metric space. The curvature tensors for the generalized affine geodesic spaces are defined by⁹

$$R_{nkm}^k = (\partial_n \bar{\Gamma}_{m i}^k - \Gamma_n^r \partial_r \bar{\Gamma}_{m i}^k) - (\partial_m \bar{\Gamma}_{i n}^k - \Gamma_m^r \partial_r \bar{\Gamma}_{i n}^k) + \bar{\Gamma}_{nr}^k \bar{\Gamma}_{m i}^r - \bar{\Gamma}_{mr}^k \bar{\Gamma}_{i n}^r \quad (2.18)$$

and

$$T_{nmi}^k = \dot{\partial}_n \bar{\Gamma}_{m i}^k, \quad (2.19)$$

where

$$\partial k(\cdot) = \frac{\partial(\cdot)}{\partial x^k}, \quad \dot{\partial}_n(\cdot) = \frac{\partial(\cdot)}{\partial(dx^n/ds)}, \quad \Gamma_m^r = \bar{\Gamma}_{m i}^r \frac{dx^i}{ds}. \quad (2.20)$$

An easy calculation shows that in our case

$$T_{mr}^k = 2 \left(\sum_{m=1}^3 \frac{dx^m}{ds} \frac{dx_m}{ds} \right)^{-2} \frac{dx_n}{ds} \bar{g}_{hr} R^k. \quad (2.21)$$

Note that both R_{nkm}^k and T_{nmi}^k depend on R^k . This is an important property of the present formulation of the equations of motion of an elastic body point, since informations about the path of the particle could be obtained solely from the informations about the stress state of the body β . This may be particularly important in the case of stress controlled motions of an elastic body, in which certain restrictions on the stress state are imposed. Then Eqs. (2.18) and (2.21) determine the restrictions on the path of \hat{X} in $L^{\hat{X}}$.

The space $L^{\hat{X}}$ coincides with the space E if $R^k = 0$. It follows from (2.7) that for initially homogeneous bodies in the absence of body forces, $R^k = 0$ if the total

covariant derivative of the deformation gradient vanishes during the motion.

3. GEOMETRY OF MOTION OF A CLASS OF DYNAMIC UNIVERSAL SOLUTIONS FOR INCOMPRESSIBLE ELASTIC BODIES

A motion $x^k = \chi^k(X^\alpha, t)$ is a dynamic universal solution⁶ for incompressible simple elastic body, if and only if, the acceleration a_k is a lamellar field with a single valued, possibly time dependent, potential¹⁰

$$a_k = \frac{\partial \xi(x^k, t)}{\partial x^k}, \quad k=1, 2, 3. \quad (3.1)$$

From (2.8) we find that

$$R^k = \frac{\partial \xi}{\partial x^s} g^{sk}, \quad k=1, 2, 3. \quad (3.2)$$

Consider a class of dynamic universal solutions, for which the acceleration potential ξ does not depend explicitly on time, i. e., $\xi = \xi(x^k)$. Then writing

$$a^k = \frac{d\dot{x}^k}{dx^m} \dot{x}^m, \quad (\dot{\cdot}) = \frac{d}{dt}(\cdot), \quad (3.3)$$

in (3.1), multiplying by dx^m , and adding, we get a Bernoullian type¹¹ of expression

$$\sum_{k=1}^3 \frac{1}{2} \dot{x}^k \dot{x}^k = \xi(x^k) + C, \quad C = \text{const.} \quad (3.4)$$

Using (3.4) we can formulate the following proposition.

Proposition: In a motion for which (3.4) holds each body point \hat{X} moves along a geodesic line in a linearly connected space $L^{\hat{X}}$ with the metric (2.9) and the con-

nection coefficients

$${}^r \bar{\Gamma}_{rk}^m = \begin{cases} m \\ r \ k \end{cases} - \frac{1}{2(\xi + C)} \xi^{,m} \bar{g}_{rk}, \quad m, r, k = 1, 2, 3, \quad (3.5)$$

$${}^r \bar{\Gamma}_{rk}^m = {}^r \bar{\Gamma}_{rk}^4 = {}^r \bar{\Gamma}_{rk}^4 = 0, \quad m, k = 1, 2, 3, 4, \quad (3.6)$$

where $\xi^{,m} = (\partial \xi / \partial x^s) g^{ms}$. Note that in (3.5) ${}^r \bar{\Gamma}_{rk}^m$ are functions of \bar{x}^1, \bar{x}^2 , and \bar{x}^3 only, so that the structure of ${}^r L^{\hat{X}}$ is simpler than that of $L^{\hat{X}}$. However ${}^r L^{\hat{X}}$ still is not a metric space.

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Variational interpolation

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In a recent article in this journal [E. T. Cheng and R. W. Conn, *J. Math. Phys.* **17**, 683 (1976)], a variational procedure was outlined to interpolate among known values of a functional of the solutions to inhomogeneous linear equations. In this paper, an alternate variational interpolation procedure for inhomogeneous equations is given. This alternate procedure utilizes the same data as the original method, but yields more accurate results. The same formalism can be applied to homogeneous equations, giving an interpolation procedure for homogeneous functionals such as eigenvalues. This refutes the conjecture of the earlier paper that a variational interpolation scheme for eigenvalues may not be possible.

I. INTRODUCTION

Cheng and Conn¹ (hereafter referred to as CC) have recently proposed a variational procedure to interpolate among known values of a functional of the solutions to inhomogeneous linear equations. To summarize the introduction to their paper, let ψ satisfy the inhomogeneous equation

$$L\psi = S, \quad (1)$$

where L is an arbitrary linear operator (the linear Boltzmann operator in the neutron transport example of CC), ψ is the dependent variable, and S is a known inhomogeneous term. Suppose one is interested not in ψ itself, but is content with knowing the inner product (S^*, ψ) , an arbitrary linear functional of the solution. (S^* is a known, arbitrary, function.) Two widely used variational principles to estimate linear functionals are those due to Roussopoulos² and Schwinger,³ given by

$$F_R[\phi, \phi^*] = (S^*, \phi) + (S, \phi^*) - (\phi^*, L\phi), \quad (2)$$

and

$$F_S[\phi, \phi^*] = (S^*, \phi)(S, \phi^*) / (\phi^*, L\phi), \quad (3)$$

where ϕ is an estimate (trial function) of ψ , and similarly ϕ^* is an estimate of the adjoint solution satisfying the adjoint equation

$$L^*\psi^* = S^*. \quad (4)$$

The well known utility of Eqs. (2) and (3) is that first order errors in the trial functions ϕ and ϕ^* lead to values of F_R and F_S which differ in second order from the functional of interest (S^*, ψ) . It should be noted that the Schwinger functional can be derived from the Roussopoulos functional by using trial functions which are the product of an amplitude and a shape function, and demanding that the resulting functional be stationary with respect to the amplitude factors.⁴ Thus the Schwinger functional is homogeneous in the trial functions ϕ and ϕ^* , as can be seen from Eq. (3), whereas the Roussopoulos functional, Eq. (2), is not. Since the Schwinger functional results from the optimization of the Roussopoulos functional over amplitudes, one would in general expect the Schwinger functional to be more accurate. Experience with these functionals bears this out in practice.

Cheng and Conn considered the problem where the operator L and/or the direct and adjoint inhomogeneous terms S and S^* depend in a known way on a set of parameters α . If $\alpha = \alpha_1$ corresponds to a reference case for which exact solutions ψ_1 and ψ_1^* are known, then either the Roussopoulos or the Schwinger functional can be used, with ψ_1 and ψ_1^* as trial functions, to estimate (to second order) the effect of changing α on the functional of interest (S^*, ψ) . These authors noted, however, that the perturbation embedded in α is often large (thus negating the second order characteristic of the usual variational principles), or that more than one reference case is appropriate. They developed a formalism based on variational techniques that allows one to interpolate between these known reference cases. In particular, for linear functionals of the solution to an inhomogeneous equation, their technique allows interpolation among an arbitrary number of reference points.

In this note, our intent is threefold: (1) for inhomogeneous equations we present an alternate formulation of variational interpolation of linear functionals which uses the same reference data and is more accurate; (2) we present an N -point interpolation scheme for eigenvalues (such a scheme eluded Cheng and Conn); and (3) we point out that while variational interpolation is very elegant, there are simpler and more straightforward approaches that may be just as accurate in certain instances. Following a brief review of the CC method, we present our alternate formulation for inhomogeneous equations and give a simple numerical example comparing the two methods. We then give the straightforward extension of our method to the eigenvalue problem, and conclude with a short discussion of the utility of variational interpolation methods.

II. REVIEW OF THE CHENG-CONN PROCEDURE FOR INHOMOGENEOUS EQUATIONS

Cheng and Conn pointed out that in using the Roussopoulos or Schwinger functional, the trial functions for ψ and ψ^* need not correspond to the same reference system. Let the equations of interest be

$$L(\alpha)\psi = S(\alpha), \quad (5)$$

$$L^*(\alpha)\psi^* = S^*(\alpha), \quad (6)$$

where α represents the known perturbation in the

operator L and the inhomogeneous terms S and S^* . Equation (6) corresponds to the functional of interest (S^*, ψ) . If α_1 and α_2 characterize two reference systems between which we wish to interpolate, we choose as trial functions ψ_1 and ψ_2^* which satisfy

$$L(\alpha_1)\psi_1 = S(\alpha_1), \quad (7)$$

$$L^*(\alpha_2)\psi_2^* = S^*(\alpha_2). \quad (8)$$

It is easily shown that, with these trial functions, both the Roussopoulos and Schwinger functionals lead to exact results for (S^*, ψ) when $\alpha = \alpha_1$ or $\alpha = \alpha_2$. For any other value of α , these functionals provide an estimate of (S^*, ψ) , the error in which is second order in the error in the trial functions.

Cheng and Conn then went further and considered the case of interpolation between an arbitrary number of reference systems. As in their paper, we illustrate their method for the case of three reference systems. Let ψ_1 and ψ_2 be exact solutions of the direct equation corresponding to parameters α_1 and α_2 , and let ψ_3^* be an exact solution to the adjoint equation when $\alpha = \alpha_3$. The CC procedure is to use in the Roussopoulos functional the trial functions

$$\phi(\alpha) = [1 - a(\alpha)]\psi_1 + a(\alpha)\psi_2, \quad (9)$$

$$\phi^*(\alpha) = b(\alpha)\psi_3^*, \quad (10)$$

and demand that the resulting functional be stationary with respect to $a(\alpha)$ and $b(\alpha)$. Having determined $a(\alpha)$ and $b(\alpha)$, Eqs. (9) and (10) are once again used in the Roussopoulos functional. The result is

$$F_{CC} = \{ (S^*, \psi_1)(\psi_3^*, L\psi_2) - (S^*, \psi_2)(\psi_3^*, L\psi_1) + (S, \psi_3^*)[(S^*, \psi_2) - (S^*, \psi_1)] / [(\psi_3^*, L\psi_2) - (\psi_3^*, L\psi_1)], \quad (11)$$

which is easily shown to give an exact value for (S^*, ψ) when $\alpha = \alpha_1$, α_2 , or α_3 . The generalization of Eq. (11) to an arbitrary number of reference systems was given by CC.

Equation (11) has characteristics of both the Schwinger and Roussopoulos functionals. It is homogeneous in the reference function ψ_3^* (as in characteristic of the Schwinger functional), but depends upon the overall amplitude of the reference functions ψ_1 and ψ_2 (as is characteristic of the Roussopoulos functional). The reason for this hybrid character of the CC functional is easily traced back to the form of the trial functions, Eqs. (9) and (10). Any change in the overall amplitude of ψ_3^* can be compensated for by a change in the coefficient $b(\alpha)$. A change in the amplitude of ψ_1 or ψ_2 , however, cannot be compensated for by changing $a(\alpha)$. That is, the amplitude of ψ_3^* has been variationally optimized, but this is not true for the amplitudes of ψ_1 and ψ_2 . We pointed out earlier that the Schwinger functional results from the Roussopoulos functional by optimizing the overall amplitude of the trial functions. The CC method is a partial extension of this procedure in which a portion of the amplitudes are optimized; i. e., a full optimization with three reference functions would require three adjustable coefficients rather than just the two $a(\alpha)$ and $b(\alpha)$. A seemingly more straight-

forward procedure would be a full extension of the derivation of the Schwinger result from the Roussopoulos result; namely, let all of the amplitudes of the reference states (trial functions) in the Roussopoulos functional be variationally optimized. The result will be a functional homogeneous in all trial functions, i. e., entirely of the Schwinger type. Not only will this result be of a more symmetric form, but it should be more accurate than the CC result since more parameters are being variationally optimized. At the same time, it is no more complex than the CC method in the sense that the same number of reference systems is being used.

III. FORMULATION FOR INHOMOGENEOUS EQUATIONS

The formulation is entirely straightforward. We assume $2N$ distinct reference systems and take as trial functions

$$\phi(\alpha) = \sum_{i=1}^N a_i(\alpha)\psi_i, \quad (12)$$

$$\phi^*(\alpha) = \sum_{i=N+1}^{2N} b_i(\alpha)\psi_i^*, \quad (13)$$

where the ψ_i and ψ_i^* satisfy

$$L(\alpha_i)\psi_i = S(\alpha_i), \quad i = 1, \dots, N, \quad (14)$$

$$L^*(\alpha_i)\psi_i^* = S^*(\alpha_i), \quad i = N+1, \dots, 2N. \quad (15)$$

Use of Eqs. (12) and (13) in the Roussopoulos functional, Eq. (2), yields, demanding that the reduced functional be stationary with respect to variations in $a_i(\alpha)$ and $b_i(\alpha)$,

$$\sum_{j=1}^N a_j(\alpha) (\psi_j^*, L(\alpha)\psi_j) = (\psi_i^*, S(\alpha)), \quad (16)$$

$$i = N+1, \dots, 2N,$$

$$\sum_{j=N+1}^{2N} b_j(\alpha) (\psi_j, L^*(\alpha)\psi_j^*) = (\psi_i, S^*(\alpha)), \quad (17)$$

$$i = 1, \dots, N.$$

These equations are to be solved for the a_i and b_i , and by Cramer's rule such solutions are just the ratio of two determinants. Using these solutions in Eqs. (12) and (13), and using these trial functions in the Roussopoulos functional gives a functional which is homogeneous with respect to all the functions ψ_i and ψ_i^* ; i. e., it is entirely of the Schwinger type. It is easily shown that this functional gives an exact result for (S^*, ψ) when $\alpha = \alpha_i$, i. e., in the reference cases. For any other value of α , this functional can be considered as a variational interpolation between the reference cases.

If we denote this functional by $F_{2N}[\phi, \phi^*; \alpha]$, we have for $N=1$

$$F_2[\phi, \phi^*; \alpha] = \frac{(S^*, \psi_1)(S, \psi_2^*)}{(\psi_2^*, L\psi_1)}, \quad (18)$$

which is just the Schwinger functional with different reference states for the direct trial function ϕ and the adjoint trial function ϕ^* . Equation (18) was first proposed, and used, by Cheng and Conn. The case $N=2$ is more interesting. We have

$$F_4 = \frac{(S^*, \psi_1)[(S, \psi_3^*)(\psi_4^*, L\psi_2) - (S, \psi_4^*)(\psi_3^*, L\psi_2)]}{(\psi_3^*, L\psi_1)(\psi_4^*, L\psi_2) - (\psi_3^*, L\psi_2)(\psi_4^*, L\psi_1)} \quad (19)$$

$$+ \frac{(S^*, \psi_2)[(S, \psi_4^*)(\psi_3^*, L\psi_1) - (S, \psi_3^*)(\psi_4^*, L\psi_1)]}{(\psi_3^*, L\psi_1)(\psi_4^*, L\psi_2) - (\psi_3^*, L\psi_2)(\psi_4^*, L\psi_1)}.$$

We see this functional is homogeneous and symmetric with respect to all four reference functions ψ_1 , ψ_2 , ψ_3^* , and ψ_4^* . This is to be contrasted with the corresponding CC result which does not enjoy this property. As remarked earlier, the CC method can be considered as a hybrid, somewhere between a Roussopoulos type functional and a Schwinger type functional. Equation (19) gives exact results for (S^*, ψ) when $\alpha = \alpha_1, \alpha_2, \alpha_3$, or α_4 , and gives second order errors for any other value of α .

Before giving an example comparing the present method with the CC procedure, it should be remarked that it is necessary in our scheme to have an equal number of direct and adjoint reference functions. If this is not the case, the reduced functional will not have a solution for the α_i and b_i . In the case of an even number of reference systems, one merely needs to use, or compute, the same number of direct solutions as adjoint solutions. However, what is the procedure to interpolate between an odd number of reference systems, say $2N - 1$? The suggestion is to use N direct solutions, $N - 1$ adjoint solutions, and an additional nonreference adjoint trial function which is arbitrary. (Although this function is arbitrary, better results will be obtained if care is taken to make this function a reasonable one.) The resulting functional F_{2N} will successfully interpolate between $2N - 1$ reference systems. To make these points clearer, we shall consider the case of an odd number of reference systems in an illustrative example.

IV. AN ILLUSTRATIVE EXAMPLE

We consider the following equation

$$-\frac{d^2\psi(x)}{dx^2} + \alpha^2\psi(x) = 1, \quad -1 \leq x \leq 1, \quad (20)$$

with boundary conditions

$$\psi(-1) = \psi(1) = 0, \quad (21)$$

and assume we are interested in the quantity

$$P \equiv \frac{\alpha^2}{2} \int_{-1}^1 dx \psi(x) = \frac{\alpha^2}{2} (S^*, \psi), \quad (22)$$

where we have defined $S^*(x) \equiv 1$. Since $S = S^*$, and the operator of Eq. (20) is self-adjoint, the entire problem is self-adjoint and we have $\psi^*(x) = \psi(x)$. We use the variational procedure of the last section to estimate (S^*, ψ) , and hence P , and compare the results with the CC procedure applied to the same problem. Physically, Eq. (20) corresponds to a simple neutron diffusion description of an infinite slab problem of thickness two, with length measured in units such that the diffusion coefficient is unity. The absorption cross section is given by α^2 , and the inhomogeneous term represents a neutron source which is independent of position. The source neutrons can either be absorbed in the slab, or leak through the faces, and the quantity P defined by

Eq. (22) is the probability of absorption. The exact solution to this problem is

$$\psi(x) = \psi^*(x) = \frac{1}{\alpha^2} \left[1 - \frac{\cosh(\alpha x)}{\cosh(\alpha)} \right]. \quad (23)$$

and thus

$$P = 1 - \frac{1}{\alpha} \tanh(\alpha). \quad (24)$$

The variational estimates will be compared to Eq. (24).

We assume three reference states, corresponding to $\alpha = 0, 1$, and ∞ . Thus we set

$$\psi_1(x) = \frac{1}{2}(1 - x^2), \quad (25)$$

$$\psi_2(x) = 1 - \frac{\cosh(x)}{\cosh(1)}, \quad (26)$$

$$\psi_3^*(x) = \lim_{\alpha \rightarrow \infty} \psi(x). \quad (27)$$

Thus both the CC method and the present procedure will give exact results for the absorption probability for $\alpha = 0, 1$, and ∞ . These three reference states can immediately be used in Eq. (11) to obtain the CC result for this problem. As discussed in the last section, however, the present scheme requires a second adjoint trial function. This simplest choice of a function which satisfies the boundary conditions might be the Dirac delta function

$$\psi_4^*(x) = \delta(x). \quad (28)$$

Equations (25)–(28) can now be used in Eq. (19) to obtain an estimate of $(1, \psi)$, and hence P , for any α . A better choice for $\psi_4^*(x)$ would probably be

$$\psi_4^*(x) = 1 - x^4, \quad (29)$$

since it not only satisfies the boundary conditions, but has the general shape of the exact solution. Equation (29), together with Eqs. (25)–(27), can then be used in Eq. (19) to obtain another variational estimate of P , the capture probability. Based upon the arguments of the last section, one would expect the results using either Eq. (28) or Eq. (29) to be superior to the CC result, with the Eq. (29) result being the best.

This *a priori* ranking is confirmed by the numerical results. For any value of α , Eq. (29) gives the best results, Eq. (28) second best, and the CC result is least accurate. Figure 1 shows these numerical results for $\alpha > 1$. The error plotted in this figure is defined as

$$\text{error} = \frac{|P_{\text{exact}} - P_{\text{approx}}|}{P_{\text{exact}}}. \quad (30)$$

We note that the Eq. (29) result has a local dip in the error in the vicinity of $\alpha = 5$. This is because the fourth trial function, Eq. (29), is actually a fairly good representation of the exact solution for this value of α . This points out the utility of taking some care in choosing the arbitrary fourth function $\psi_4^*(x)$.

V. FORMULATION FOR EIGENVALUES

The Rayleigh quotient is a homogeneous functional which is widely used to estimate eigenvalues. Cheng and Conn pointed out that by using different reference states for the direct and adjoint trial functions, one can

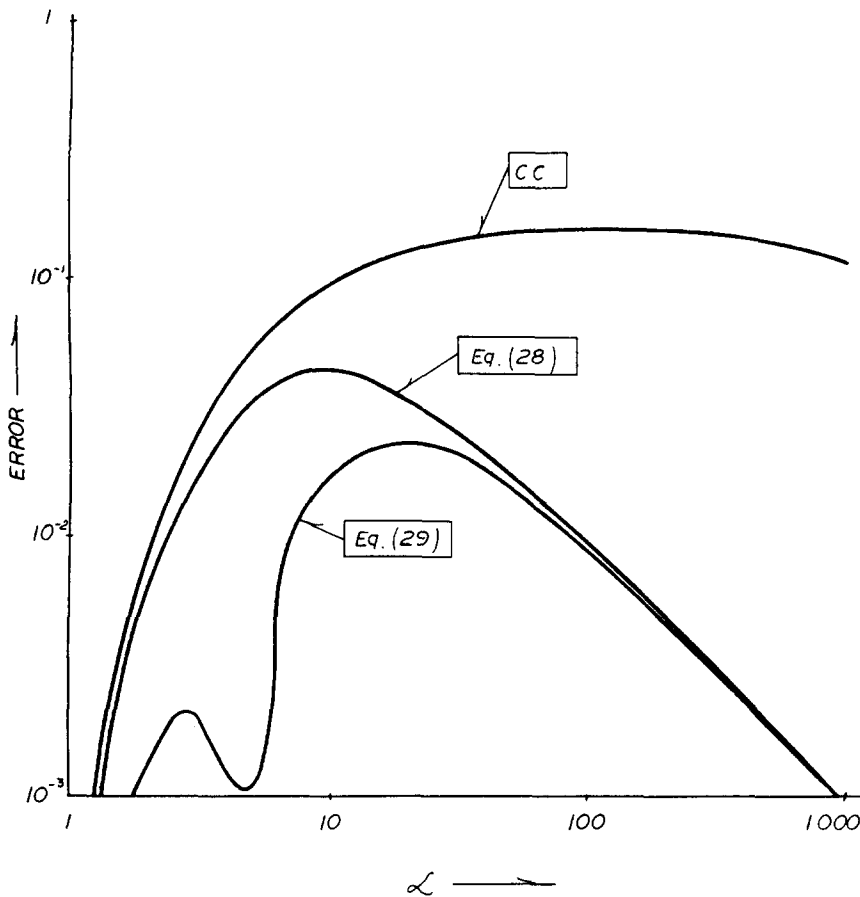


FIG. 1. The error in the capture probability versus the absorption cross section.

use the Rayleigh quotient to interpolate between the known eigenvalues of two reference states. However, they were unable, and conjectured that it may be impossible, to find a variational interpolation scheme involving more than two reference states. Using the same methods as we have employed for inhomogeneous equations, we find it is possible to construct an interpolation scheme for eigenvalues involving an arbitrary number of reference states.

We consider the eigenvalue equation

$$L(\alpha)\psi = \Lambda F(\alpha)\psi, \quad (31)$$

and the corresponding adjoint equation

$$L^*(\alpha)\psi^* = \Lambda F^*(\alpha)\psi^*, \quad (32)$$

where Λ is the eigenvalue and L and F are linear operators. (For notational simplicity, we do not employ an index to distinguish the various modes.) The Roussopoulos functional for these equations is

$$F[\phi, \phi^*, \lambda] = (\phi^*, L\phi - \lambda F\phi), \quad (33)$$

where ϕ and ϕ^* are trial functions for ψ and ψ^* , and λ is a trial scalar for the eigenvalue Λ .⁵ The procedure is to use trial functions of the form

$$\phi(\alpha) = \sum_{i=1}^N a_i(\alpha)\psi_i, \quad (34)$$

$$\phi^*(\alpha) = \sum_{i=N+1}^{2N} b_i(\alpha)\psi_i^*, \quad (35)$$

where, just as in the inhomogeneous case, ψ_i and ψ_i^*

represent exact solutions for the i th reference state. These trial functions are used in Eq. (33) and the resulting functional rendered stationary with respect to independent and arbitrary variations in the $a_i(\alpha)$ and $b_i(\alpha)$. The result is the set of inhomogeneous equations

$$\sum_{j=1}^N a_j(\alpha)(\psi_i^*, L(\alpha)\psi_j) = \lambda \sum_{j=1}^N a_j(\alpha)(\psi_i^*, F(\alpha)\psi_j), \quad (36)$$

$$i = N+1, \dots, 2N,$$

$$\sum_{j=N+1}^{2N} b_j(\alpha)(\psi_i, L^*(\alpha)\psi_j^*) = \lambda \sum_{j=N+1}^{2N} b_j(\alpha)(\psi_i, L^*(\alpha)\psi_j^*), \quad (37)$$

$$i = 1, \dots, N.$$

Equation (36) represents N homogeneous equations for the $a_i(\alpha)$. For these equations to have a nontrivial solution, the coefficient determinant must vanish, i. e.,

$$\begin{vmatrix} (\psi_{N+1}^*, L\psi_1 - \lambda F\psi_1) & \dots & (\psi_{N+1}^*, L\psi_N - \lambda F\psi_N) \\ \vdots & & \vdots \\ (\psi_{2N}^*, L\psi_1 - \lambda F\psi_1) & \dots & (\psi_{2N}^*, L\psi_N - \lambda F\psi_N) \end{vmatrix} = 0. \quad (38)$$

The same statement holds true for the N equations given by Eq. (37), and this leads again to the determinant given by Eq. (38). Equation (38), when solved for λ , is the extension of the Rayleigh quotient to an arbitrary number of reference systems. It is clear from Eq. (38) that one obtains the exact solution, $\lambda = \Lambda$, when $\alpha = \alpha_1, \alpha_2, \dots$, or α_{2N} , and it is easily shown that Eq. (38) estimates Λ with second order

errors for any other value of α . The usual Rayleigh quotient is recovered when $N=1$. In this case, the determinant has only one element and we find, solving for λ ,

$$\lambda = \frac{(\psi_2^*, L\psi_1)}{(\psi_2^*, F\psi_1)}. \quad (39)$$

This is the usual Rayleigh quotient involving two different reference states, as suggested by Cheng and Conn. For $N=2$ we have

$$\begin{aligned} & [(\psi_3^*, L\psi_1) - \lambda(\psi_3^*, F\psi_1)][(\psi_4^*, L\psi_2) - \lambda(\psi_4^*, F\psi_2)] \\ & = [(\psi_3^*, L\psi_2) - \lambda(\psi_3^*, F\psi_2)][(\psi_4^*, L\psi_1) - \lambda(\psi_4^*, F\psi_1)], \end{aligned} \quad (40)$$

which is a quadratic in λ . One solution for λ corresponds to the interpolation for the mode of interest between the reference states α_1 , α_2 , α_3 , and α_4 , whereas the second solution is a (probably crude) estimate of an eigenvalue corresponding to another mode.

VI. CONCLUDING REMARKS

In this paper we have shown that the original idea of Cheng and Conn to use variational methods to interpolate between known reference states can be extended. For linear functionals of the solution to inhomogeneous equations, this extension amounted to an alternate way of using the reference states which, because it allowed more freedom in combining these states, led to more accurate results. For eigenvalues, the extension was made to more than two reference states. The formalism employed as the starting point was the well-known Roussopoulos functional, using trial functions whose components are the product of shape functions (the reference solutions) and amplitude factors. The amplitude factors are variationally optimized to achieve the mixing, or interpolation, of the reference solutions. Although this paper, as well as the paper of Cheng and Conn, dealt specifically with linear functionals for inhomogeneous equations and eigenvalues for homogeneous equations, the same formalism could be used to develop variational interpolation formulas for arbitrary functionals of interest for both inhomogeneous and homogeneous equations. One would use the same type of trial functions, but start with, rather than the Roussopoulos functional, the generalization of the Roussopoulos functional appropriate to the functional of interest. This generalization of the Roussopoulos functional for estimating an arbitrary functional has previously been reported for both homogeneous⁵ and inhomogeneous⁶ equations.

Two other concluding comments seem in order. First, we remarked earlier that the present extension of the CC method for inhomogeneous equations is more accurate, but no more complex, than the original CC method. This assertion concerning complexity is true

in the sense that in both instances the same reference states are involved, and in most problems it is the generation of the reference solutions that constitutes most of the complexity. However, once the reference solutions are known, clearly our method is algebraically more complex than the CC method because it involves the calculation of more coefficients $a_i(\alpha)$ and $b_i(\alpha)$. It is just this fact that more coefficients are used, which means more flexibility for the variational method to interpolate, that leads to the increased accuracy.

Finally, the two characteristics of any variational interpolation scheme that make it attractive are: (i) interpolation is possible between an arbitrary number of reference states; and (ii) errors are second order in the inaccuracies of the trial functions. The first characteristic is shared by most interpolation schemes, e.g., fitting $N+1$ points with an N th order polynomial. Further, if the perturbation embedded in α is large (if the reference states are far apart), then the fact that the errors in variational interpolation are of second order is of no particular *a priori* advantage. Second order errors may be as large, or larger, than first order errors. This observation leads to the second comment. For large perturbations, variational interpolation, while mathematically appealing, may be no more accurate than a simpler method such as a polynomial, or other functional form, fit. Accordingly, one should consider the variational interpolation schemes discussed in this paper as a technique to complement, but not necessarily replace, other interpolation schemes.

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Exact propagators for quadratic Hamiltonians^{a)}

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The problem of finding the exact propagator for a given quadratic Hamiltonian is presented as an initial-value problem — a form suitable for both analytic and numerical computation. We illustrate the method by finding the propagator for (a) the Hamiltonian with constant coefficients and (b) and (c) Hamiltonians associated with damped harmonic motion.

1. INTRODUCTION

It is well known that the problem of finding the exact propagator for a given quadratic Hamiltonian can essentially be solved. Perhaps the most natural approach to the subject is provided by the path-integral method. By expanding all possible paths around the classical path connecting the points (x_1, t_1) and (x_2, t_2) , Feynman was able to show that the propagator in this case factors out into

$$K(x_2, t_2; x_1, t_1) = F(t_2 - t_1) \cdot \exp \frac{i}{\hbar} S_{c1}(x_2, t_2; x_1, t_1),$$

where $S_{c1}(x_2, t_2; x_1, t_1)$ is the classical action, calculated along the classical path, and F is a modulating factor depending on the time interval alone.¹ Thus, in order to calculate the propagator K , one first has to solve the classical equation of motion subject to the boundary condition that the particle goes through the endpoints at the specified times, then calculate $S_{c1} = \int_{t_1}^{t_2} L(x, \dot{x}, t) dt$, and, finally, devise a method to determine the modulating factor F . In the unfortunate case, when the classical equation of motion does not lend itself to analytic solution, one may be confronted with a formidable numerical problem.

In this paper, we show how to formulate the problem of finding K as an initial-value problem, suitable for both analytic and numerical computation. In particular, the modulating factor F is completely determined. We shall illustrate our method by solving three cases, two of which pertain to damped harmonic motion—a subject of some recent interest.²

2. INITIAL VALUE FORMULATION

In this section we shall work in one dimension. An example in two dimensions is worked out in the next section. Given the Hamiltonian

$$H(x, p, t) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 p + \alpha_4 p^2 + \alpha_5 x p + \alpha_5^* p x,$$

where, in general $\alpha_i = \alpha_i(t)$, we are asked to solve the Schrödinger equation

$$i\hbar \frac{\partial K}{\partial t} = HK \quad (1a)$$

subject to the initial condition

$$K(x, t; x', 0) \underset{t \rightarrow 0}{\sim} \delta(x - x'). \quad (1b)$$

In what follows we shall shorten the notation by suppressing the explicit dependence on x' . Thus, for example, $K(x, t; x', 0) \equiv K(x, t)$. We shall seek a solution of the form

$$K(x, t) = F(t) \cdot \exp\left(\frac{i}{\hbar} S(x, t)\right). \quad (2)$$

Substituting this expression in Eq. (1), we obtain

$$i\hbar \left(\frac{\dot{F}}{F} + \alpha_4 \frac{\partial^2 S}{\partial x^2} + \alpha_5^* \right) = \frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}, t\right). \quad (3)$$

We now try the following ansatz,

$$\frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}, t\right) = 0, \quad (4)$$

with

$$S(x, t) = a(t) + b(t)x + c(t)x^2, \quad (5)$$

and

$$\frac{\dot{F}}{F} + \alpha_4 \frac{\partial^2 S}{\partial x^2} + \alpha_5^* = 0. \quad (6)$$

The Hamilton–Jacobi equation yields

$$\dot{a} + \alpha_0 + \alpha_3 b + \alpha_4 b^2 = 0, \quad (7a)$$

$$\dot{b} + \alpha_1 + (\alpha_5 + \alpha_5^*)b + 2\alpha_3 c + 4\alpha_4 b c = 0, \quad (7b)$$

$$\dot{c} + \alpha_2 + 2(\alpha_5 + \alpha_5^*)c + 4\alpha_4 c^2 = 0, \quad (7c)$$

while Eq. (6) gives

$$\dot{F}/F = -(2\alpha_4 c + \alpha_5^*).$$

Hence,

$$F(t) = F(t_0) \exp\left[-\int_{t_0}^t (2\alpha_4 c + \alpha_5^*) dt'\right]. \quad (8)$$

The appropriate initial conditions for Eqs. (7) can be obtained by invoking the representation of the delta function as a limiting form of a free propagator

$$\frac{1}{(\pi\lambda t)^{1/2}} \exp\left[-\frac{(x-x')^2}{\lambda t}\right] \underset{t \rightarrow 0}{\sim} \delta(x-x'), \quad (9)$$

where λ is a constant. With this representation we have (as $t \rightarrow 0$)

$$K = F(t) \exp\left(\frac{i}{\hbar} (a + bx + cx^2)\right) \sim (\pi\lambda t)^{-1/2} \exp\left[-(x-x')^2/(\lambda t)\right]. \quad (10)$$

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Hence,

$$b \sim -2i\hbar x' / (\lambda t) \quad \text{and} \quad c \sim i\hbar / (\lambda t). \quad (11)$$

Inserting these relations into Eqs. (7), we obtain [assuming $\alpha_i(t)$ regular at $t=0$]

$$\lambda = 4i\hbar\alpha_4(0), \quad (12)$$

$$c \sim 1/[4\alpha_4(0)t], \quad (13a)$$

$$b \sim -x' / [2\alpha_4(0)t], \quad (13b)$$

and

$$a \sim x'^2 / [4\alpha_4(0)t]. \quad (13c)$$

Equations (13a) and (13b) determine $c(t)$ and $b(t)$ uniquely. To fix $a(t)$, we have to supply the integration constant in Eq. (7a). As shown in the Appendix, this constant is given by

$$\alpha_0 = \{ [4\alpha_4(0) \operatorname{Re}\alpha_5(0) - \dot{\alpha}_4(0)] x'^2 + 4\alpha_4(0) \alpha_3(0) x' \} / (8\alpha_4^2(0)), \quad (13d)$$

where

$$a \sim x'^2 / (4\alpha_4(0)t) + a_0. \quad (13e)$$

Finally, from Eqs. (8), (10), (12), and (13) we have

$$F(t_0) = \lim_{t \rightarrow 0} \exp \left[\int_{t_0}^t (2\alpha_4 c + \alpha_5^*) dt' \right] / (4i\hbar\pi\alpha_4 t)^{1/2}. \quad (14)$$

Equations (7), (13), (8), and (14) constitute our initial value problem for the determination of the propagator.

The general solution of Eq. (7c) (Riccati's equation) is, of course, not known. However, if a particular solution $c = c_1$ can be guessed, the substitution $c = c_1 + 1/z$ with $z(0) = 0$ leads to a solvable linear equation. Once $c(t)$ is determined, the linear equations for $b(t)$ and $a(t)$ can be solved and the modulating function $F(t)$ can be calculated. In general, however, Eq. (7c) with the initial condition (13c) has to be solved numerically. Note that $c(t)$ is independent of x' and can be calculated "once and for all."

3. EXAMPLES

A. Hamiltonian with constant coefficients

In the case where α_i are time independent, the solution for the propagator can be readily found. A particular solution of Eq. (7c) is

$$c_1 = (-2 \operatorname{Re}\alpha_5 + i\Omega) / (4\alpha_4), \quad (15)$$

with

$$\Omega = 2[\alpha_2\alpha_4 - (\operatorname{Re}\alpha_5)^2]^{1/2}. \quad (16)$$

Using this solution, we obtain after a somewhat lengthy but straightforward calculation

$$c = [-2 \operatorname{Re}\alpha_5 \sin\Omega t + \Omega \cos\Omega t] / (4\alpha_4 \sin\Omega t), \quad (17)$$

$$b = [-x'\Omega^2 + 2\beta(\cos\Omega t - 1) - \alpha_3\Omega \sin\Omega t] / (2\alpha_4\Omega \sin\Omega t), \quad (18)$$

with

$$\beta = (\alpha_1\alpha_4 - \alpha_3 \operatorname{Re}\alpha_5), \quad (19)$$

$$a = At - (B - C \cos\Omega t) / (\Omega \sin\Omega t) + x'(\alpha_3 + x' \operatorname{Re}\alpha_5) / (2\alpha_4), \quad (20)$$

with

$$A = [4\beta^2 + (\alpha_3^2 - 4\alpha_0\alpha_4)\Omega^2] / (4\alpha_4\Omega^2),$$

$$B = \beta(x'\Omega^2 + 2\beta) / (\alpha_4\Omega^2), \quad (21)$$

$$C = [(x'\Omega^2 + 2\beta)^2 + 4\beta^2] / (4\alpha_4\Omega^2),$$

and

$$F(t) = \exp(i \operatorname{Im}\alpha_5 t) [\Omega / (4\pi i \hbar \alpha_4 \sin\Omega t)]^{1/2}. \quad (22)$$

Thus, for the harmonic oscillator we have $\alpha_0 = \alpha_1 = \alpha_3 = \alpha_5 = 0$, $\alpha_2 = m\omega^2/2$, and $\alpha_4 = 1/(2m)$, yielding

$$a = \frac{1}{2} m \omega x'^2 \cos\omega t / \sin\omega t,$$

$$b = -m\omega x' / \sin\omega t,$$

$$c = \frac{1}{2} m \omega \cos\omega t / \sin\omega t,$$

$$F = [m\omega / (2\pi i \hbar \sin\omega t)]^{1/2}$$

—a well-known result.¹

B. Damped harmonic oscillator

The damped harmonic oscillator satisfies

$$\ddot{x} + 2\gamma\dot{x} + \omega^2 x = 0. \quad (23)$$

A time dependent Hamiltonian yielding this equation of motion is given by

$$H(t) = \frac{p^2}{2m} \exp(-2\gamma t) + \frac{1}{2} m \omega^2 x^2 \exp(2\gamma t). \quad (24)$$

We therefore have $\alpha_0 = \alpha_1 = \alpha_3 = \alpha_5 = 0$, and $\alpha_2 = \frac{1}{2} m \omega^2 \exp(2\gamma t)$, $\alpha_4 = (1/2m) \exp(-2\gamma t)$. A particular solution of Eq. (7c) in this case is

$$c_1 = \frac{1}{2} m (-\gamma + i\Omega) \exp(2\gamma t) \quad (25)$$

with

$$\Omega = (\omega^2 - \gamma^2)^{1/2}. \quad (26)$$

Using this particular solution, we obtain

$$a = \frac{1}{2} m \Omega x'^2 \cos\Omega t / \sin\Omega t + \frac{1}{2} m \gamma x'^2, \quad (27)$$

$$b = -m\Omega x' \exp(\gamma t) / \sin\Omega t, \quad (28)$$

$$c = \frac{1}{2} m \exp(2\gamma t) (\Omega \cos\Omega t - \gamma \sin\Omega t) / \sin\Omega t, \quad (29)$$

and

$$F = \exp(\gamma t / 2) [m\Omega / (2\pi i \hbar \sin\Omega t)]^{1/2}. \quad (30)$$

Setting $\gamma = 0$, the corresponding expressions for the free harmonic oscillator are recovered.

C. Feshbach's Hamiltonian

A time independent Hamiltonian tailored to yield the damped harmonic oscillator equation of motion, has been introduced by Feshbach.^{2,3} The trick is to couple the oscillator with another oscillator satisfying the time reversed equation of motion. This example will give us an opportunity to apply our method to a two-dimensional problem. With Ω defined by Eq. (26), Feshbach's Hamiltonian reads

$$H = \frac{1}{m} p_x p_y + \gamma (y p_y - x p_x) + m\Omega^2 xy. \quad (31)$$

The corresponding equations of motion are

$$\ddot{x} + 2\gamma\dot{x} + \omega^2 x = 0 \quad (32a)$$

$$\ddot{y} - 2\gamma\dot{y} + \omega^2 y = 0. \quad (32b)$$

Introducing the transformation

$$x = 2^{-1/2}(x_1 + x_2), \quad y = 2^{-1/2}(x_1 - x_2), \quad (33)$$

we secure

$$H = \left(\frac{P_1^2}{2m} + \frac{1}{2}m\Omega^2 x_1^2 \right) - \left(\frac{P_2^2}{2m} + \frac{1}{2}m\Omega^2 x_2^2 \right) - \gamma(x_2 p_1 + x_1 p_2). \quad (34)$$

Note that the unperturbed Hamiltonian is the *difference* rather than the sum of the two free Hamiltonians. We shall now proceed to calculate the propagator $K(x_1, x_2, t) \equiv K(x_1, x_2, t; x_1', x_2', 0)$. Again, we seek a solution of the form (2). The Schrödinger equation yields in this case.

$$i\hbar \left(\frac{\dot{F}}{F} + \frac{1}{2m} \frac{\partial^2 S}{\partial x_1^2} - \frac{1}{2m} \frac{\partial^2 S}{\partial x_2^2} \right) = \frac{\partial S}{\partial t} + H \left(x_1, x_2, \frac{\partial S}{\partial x_1}, \frac{\partial S}{\partial x_2} \right). \quad (35)$$

The ansatz

$$\frac{\partial S}{\partial t} + H \left(x_1, x_2, \frac{\partial S}{\partial x_1}, \frac{\partial S}{\partial x_2} \right) = 0 \quad (36)$$

with

$$s = a + bx_1 + cx_2 + dx_1^2 + ex_2^2 + fx_1x_2 \quad (37)$$

and

$$\frac{\dot{F}}{F} + \frac{1}{2m} \frac{\partial^2 S}{\partial x_1^2} - \frac{1}{2m} \frac{\partial^2 S}{\partial x_2^2} = 0 \quad (38)$$

give:

$$\dot{a} + \frac{1}{2}(b^2 - c^2)/m = 0, \quad (39a)$$

$$\dot{b} + (2bd - cf)/m - \gamma c = 0, \quad (39b)$$

$$\dot{c} + (bf - 2ce)/m - \gamma b = 0, \quad (39c)$$

$$\dot{d} + \frac{1}{2}(4d^2 - f^2)/m + \frac{1}{2}m\Omega^2 - \gamma f = 0, \quad (39d)$$

$$\dot{e} + \frac{1}{2}(f^2 - 4e^2)/m - \frac{1}{2}m\Omega^2 - \gamma f = 0, \quad (39e)$$

$$\dot{f} + (2df - 2ef)/m - 2\gamma(d + e) = 0, \quad (39f)$$

and

$$\dot{F}/F = -(d - e)/m,$$

yielding

$$F(t) = F(t_0) \exp \left[-\frac{1}{m} \int_{t_0}^t (d - e) dt' \right]. \quad (40)$$

Similarly, using the relation

$$K = F(t) \exp \left[\frac{i}{\hbar} (a + bx_1 + cx_2 + dx_1^2 + ex_2^2 + fx_1x_2) \right] \\ \underset{t \rightarrow 0}{\sim} (\pi\lambda_1 t)^{-1/2} \exp \left(-\frac{(x_1 - x_1')^2}{\lambda_1 t} \right) \cdot (\pi\lambda_2 t)^{-1/2} \exp \left(-\frac{(x_2 - x_2')^2}{\lambda_2 t} \right) \quad (41)$$

and the differential equations (39), the following initial conditions can be derived (for $t \rightarrow 0$):

$$a \sim \frac{1}{2}m(x_1'^2 - x_2'^2)/t, \\ b \sim -mx_1'/t, \quad c \sim mx_2'/t, \\ d \sim \frac{1}{2}m/t, \quad e \sim -\frac{1}{2}m/t, \\ f(0) = 0, \quad (42)$$

and

$$F(t_0) = \lim_{t \rightarrow 0} \frac{m}{2\pi\hbar t} \exp \left(\frac{1}{m} \int_{t_0}^t (d - e) dt' \right). \quad (43)$$

Inspection of the differential equations and the initial conditions reveal that

$$f(t) \equiv 0, \quad e(t) = -d(t). \quad (44)$$

Also, we note that $d_1 = im\Omega/2$ is a particular solution of Eq. (39d). Proceeding to solve the remaining equations we secure

$$d = \frac{1}{2}m\Omega \cos\Omega t / \sin\Omega t, \quad (45)$$

$$c = -m\Omega(x_1' \sinh\gamma t - x_2' \cosh\gamma t) / \sin\Omega t, \quad (46)$$

$$b = -m\Omega(x_1' \cosh\gamma t - x_2' \sinh\gamma t) / \sin\Omega t, \quad (47)$$

$$a = \frac{1}{2}m\Omega(x_1'^2 - x_2'^2) \cos\Omega t / \sin\Omega t, \quad (48)$$

and

$$F = m\Omega / (2\pi\hbar \sin\Omega t). \quad (49)$$

It is easy to check that the initial condition $K \sim \delta(x_1 - x_1') \delta(x_2 - x_2')$ is indeed satisfied by the solution above. The peculiarities of Feshbach's Hamiltonian are again manifested in the limit of no-interaction. Letting $\gamma \rightarrow 0$ we obtain [in accordance with the minus sign in Eq. (34)],

$$K(x_1, x_2, t; x_1', x_2', 0) \underset{\gamma \rightarrow 0}{\rightarrow} K_0(x_1, t; x_1', 0) \cdot K_0^*(x_2, t; x_2', 0), \quad (50)$$

where K_0 is the propagator for the free harmonic oscillator. This suggests that K should be interpreted as the amplitude for particle 1 to go from x_1' at $t=0$ to x_1 at time t , while particle 2 proceeds from x_2 at time t to x_2' at $t=0$. An alternative derivation of this propagator, in the occupation number representation, can be found in Ref. 2.

4. DISCUSSION

We have seen above how, in the case of quadratic Hamiltonians, one can bypass the equations of motion and obtain the action directly as a solution of an initial-value problem. Though we have concentrated on one-dimensional Hamiltonians, it is clear that the method can be applied to higher dimensions.

It is perhaps interesting to note that once the initial-value problem has been solved, the classical path can be regained by an additional quadrature. We shall demonstrate this point for a somewhat limited class of Hamiltonians, namely, those with velocity independent potentials. Thus, consider the Hamiltonian

$$H = \alpha_4 p^2 + \alpha_0 + \alpha_1 x + \alpha_2 x^2, \quad (51)$$

where, in general, $\alpha_i = \alpha_i(t)$. The corresponding equation of motion,

$$\ddot{x} - (\dot{\alpha}_4/\alpha_4)\dot{x} + 2\alpha_4(\alpha_1 + 2\alpha_2x) = 0, \quad (52)$$

can be written as a first order equation, namely,

$$\frac{d}{dt} \left(\frac{1}{2\alpha_4} \dot{x} - 2cx \right) + 4\alpha_4c \left(\frac{1}{2\alpha_4} \dot{x} - 2cx \right) = -\alpha_1, \quad (53)$$

where $c(t)$ satisfies Eq. (7c). Equation (53) for the quantity

$$b = \frac{1}{2\alpha_4} \dot{x} - 2cx \quad (54)$$

coincides with Eq. (7b). Thus, given $b(t)$ and $c(t)$ as determined by Eqs. (7c), (13c), (7b), and (13b), the linear equation (54) can be solved for $x(t)$,

$$x(t) = \exp\left[-\int_t^T 4\alpha_4c dt'\right] \left\{ x - \int_t^T 2\alpha_4b \times \exp\left[\int_{t'}^T 4\alpha_4c dt''\right] dt' \right\}. \quad (55)$$

In the above, we have used $x(T) = x$. It is not difficult to check [using Eq. (13b) and (13c)] that the trajectory (55) satisfies

$$x(t) \xrightarrow{t \rightarrow 0} x'. \quad (56)$$

Thus, $x(t)$ as given by Eq. (55) is the classical path passing through the end point x' and x at times $t=0$ and $t=T$.

The Lagrangian for the system is given by

$$L = p\dot{x} - H = \dot{x}^2/(4\alpha_4) - \alpha_0 - \alpha_1x - \alpha_2x^2. \quad (57)$$

Using Eqs. (7) and (54) we have

$$\begin{aligned} L &= [\dot{x}(b + 2cx) - \alpha_4(b + 2cx)^2] + (\dot{a} + \alpha_4b^2) \\ &\quad + (\dot{b} + 4\alpha_4bc)x + (\dot{c} + 4\alpha_4c^2)x^2 \\ &= \frac{d}{dt} (a + bx + cx^2). \end{aligned}$$

Thus

$$S_{cl} \equiv \int_0^T L dt = \lim_{t_0 \rightarrow 0} [S(x(T), T) - S(x(t_0), t_0)]. \quad (58)$$

Introducing $x(T) = x$, $x(0) = x'$, and using the initial values (13) and Eq. (A4), we obtain

$$S_{cl}(x, T; x', 0) = S(x, T) \equiv S(x, T; x', 0). \quad (59)$$

The classical action is therefore that solution of the Hamilton–Jacobi equation, which satisfies the initial condition (13), namely,

$$S_{cl}(x, T; x', 0) \underset{T \rightarrow 0}{\sim} \frac{1}{4\alpha_4(0)} \frac{(x - x')^2}{T} \equiv S_{cl}^{free}. \quad (60)$$

In the WKB approximation (which should be exact for quadratic Hamiltonians), the modulating factor F is explicitly given by⁴

$$F = \left(\frac{\partial^2 S}{\partial x \partial x'} \right) / (-2\pi i \hbar)^{1/2}. \quad (61)$$

This is a useful expression provided $S_{cl}(x, t; x', 0)$ is known analytically. Indeed, using Eqs. (4), (5), and

(13), one can check that the WKB expression (61) satisfies the differential equation (6) together with the initial condition

$$F \underset{t \rightarrow 0}{\sim} (4\pi i \hbar \alpha_4(0)t)^{-1/2}$$

as long as the coefficient α_5 in the Hamiltonian is real. The phase of the WKB expression is wrong for $\alpha_5 \neq \alpha_5^*$. Instead one has

$$F = \exp(i \int_0^t \text{Im} \alpha_5 dt') \left(\frac{\partial^2 S}{\partial x \partial x'} / (-2\pi i \hbar) \right)^{1/2}. \quad (62)$$

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APPENDIX

Equation (7a) determines $a(t)$ up to a constant. In order to establish the missing constant, we shall need the coefficients b_0 and c_0 in the expansion

$$\begin{aligned} b &\sim -2x' / [4\alpha_4(0)t] + b_0, \\ c &\sim 1 / [4\alpha_4(0)t] + c_0. \end{aligned} \quad (A1)$$

Substituting the above expansion in (7b) and (7c), we obtain

$$\begin{aligned} b_0 &= x' \dot{\alpha}_4(0) / [4\alpha_4^2(0)] - \alpha_3(0) / [2\alpha_4(0)], \\ c_0 &= -\{\text{Re} \alpha_5(0) / [2\alpha_4(0)] + \dot{\alpha}_4(0) / [8\alpha_4^2(0)]\}. \end{aligned} \quad (A2)$$

Thus, with

$$a \sim x'^2 / [4\alpha_4(0)t] + a_0 \quad (A3)$$

we have

$$\begin{aligned} K &= F(t) \exp[(i/\hbar)(a + bx + cx^2)] \\ &\sim \delta(x - x') \exp[(i/\hbar)(a_0 + b_0x + c_0x^2)]. \end{aligned}$$

In order for the right-hand side to reduce to $\delta(x - x')$, the exponent $(a_0 + b_0x + c_0x^2)$ must be a multiple of $(x - x')$. Hence,

$$a_0 = -(b_0x' + c_0x'^2). \quad (A4)$$

¹R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

²H. Feshbach and Y. Tikochinsky, "Quantization of the damped harmonic oscillator," *Rabi Festschrift* (in press).

³P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953), p. 298.

⁴See, for example, M. K. Berry and K. E. Mount, *Rep. Prog. Phys.* **35**, 315 (1972), and references therein.

Multiple density correlation functions for inhomogeneous systems^{a)}

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In applying the method of correlated basis functions to inhomogeneous systems such as electrons in a solid, in systems bounded by surfaces, and in systems with impurities, matrix elements of multiple density fluctuation operators are needed. These are the multiple density correlation functions. We evaluate these functions in the convolution approximation and express them in usable forms.

I. INTRODUCTION

In variational calculations for interacting quantum liquids and solids, correlated wavefunctions have made some rather impressive contributions.^{1,2} While this is particularly true for calculations on homogeneous systems, recent progress in treating certain classes of surface problems³ encourages us to explore further the applicability of correlated wavefunctions to many inhomogeneous systems. Among those considered are surfaces of liquid ³He and nuclear matter, inhomogeneous electron liquids, impurities in solids, exciton droplets, and atomic systems.

By correlated wavefunctions, we mean wavefunctions which take into account the more important correlation effects. In particular, one could modify the Slater determinant, D , with a Jastrow factor,

$$\psi = D \prod_{i < j} f(\mathbf{r}_i, \mathbf{r}_j), \quad (1)$$

to account for pair correlations. If the pairwise interaction between the particles contains a strong repulsive core, $f(\mathbf{r}_i, \mathbf{r}_j)$ can be chosen to diminish rapidly with $r_{ij} \equiv |\mathbf{r}_i - \mathbf{r}_j|$. Thus the Jastrow factor $\prod_{i < j} f(\mathbf{r}_i, \mathbf{r}_j)$ serves to discourage overlap of the cores and makes the wavefunction much more realistic.

In the case of homogeneous systems, the elements of D are plane waves (with spin functions for fermions), and momentum is a good quantum number. The matrix elements connecting correlated wavefunctions involve simple Fourier transforms of $f(r_{ij})$ and Kronecker deltas. They are not easy to calculate, but are still manageable with the help of appropriate approximation schemes. For inhomogeneous systems, D represents antisymmetrized products of single particle wavefunctions. The matrix elements become more complicated. We intend to show in this paper that, at least in the convolution approximation, they can still be calculated and expressed in usable forms.

To be specific, we shall write down the relevant

equations for an inhomogeneous electron liquid and identify the required matrix elements.

In this model, we assume a static lattice structure for the ions, so that the ion variables reduce to constant lattice vectors \mathbf{R}_α , $\alpha = 1, 2, \dots, N$. There are N electrons moving in a volume Ω consistent with the lattice vectors \mathbf{R}_α . The electron coordinates are denoted by \mathbf{r}_i , $i = 1, 2, \dots, N$. The electron density is represented by a function $n(\mathbf{r})$, and the mean density is given by $\rho \equiv N/\Omega \equiv (1/\Omega) \int n(\mathbf{r}) d\mathbf{r}$. The Hamiltonian for the electron system is then given by

$$H = \sum_{i=1}^N h_i + \sum_{i < j}^N v(r_{ij}) - \frac{1}{2} N \rho v_0, \quad (2)$$

where

$$h_i = \frac{-\hbar^2}{2m} \nabla_i^2 + V(\mathbf{r}_i), \quad (3)$$

$$V(\mathbf{r}_i) = \sum_{\alpha=1}^N v(|\mathbf{r}_i - \mathbf{R}_\alpha|), \quad (4)$$

and

$$v(r) = e^2/r. \quad (5)$$

In Eq. (2) v_0 denotes the Fourier transform of the Coulomb potential in the long wavelength limit. Thus the last term in Eq. (2) takes out the electron self-energy.

Generalizing our earlier work⁴ on the homogeneous electron liquid, an appropriate variational wavefunction will still take the form (1), except that D now represents a determinant made up of Bloch function elements and spin functions. For simplicity, we make the approximation that $f(\mathbf{r}_i, \mathbf{r}_j)$ be central, and write

$$\psi = D \cdot \prod_{i < j}^N f(r_{ij}) \equiv D \cdot \left\{ \exp \sum_{i < j}^N \frac{1}{2} u(r_{ij}) \right\}, \quad (6)$$

$$= D \cdot \left[\exp \left(\frac{1}{4\Omega} \sum_{\mathbf{k}} u(k) (\rho_{\mathbf{k}} \rho_{-\mathbf{k}} - N) \right) \right], \quad (7)$$

where

$$\rho_{\mathbf{k}} = \sum_{i=1}^N \exp(ik \cdot \mathbf{r}_i), \quad (8)$$

and

$$u(k) = \int u(r) \exp(ik \cdot \mathbf{r}) d\mathbf{r}. \quad (9)$$

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With respect to such a correlated wavefunction we must now evaluate the energy expectation value,

$$\langle H \rangle = \sum_{i=1}^N \langle h_i \rangle + \sum_{\substack{i < j \\ =1}} \langle v(r_{ij}) \rangle - \frac{1}{2} N \rho v_0, \quad (10)$$

where

$$\langle O \rangle = \frac{\sum_{\{\sigma\}} \int \psi^* O \psi d\mathbf{r}_1 \cdots d\mathbf{r}_N}{\sum_{\{\sigma\}} \int \psi^* \psi d\mathbf{r}_1 \cdots d\mathbf{r}_N} \quad (11)$$

for any operator O . After several steps of integration by parts and algebraic manipulation, we find

$$\begin{aligned} \langle H \rangle = & \sum_{i=1}^N \epsilon_i - \frac{\hbar^2}{8m\Omega^2} \sum_{\mathbf{k}, 1} u(k) u(l) \mathbf{k} \cdot \mathbf{l} \langle \rho_{\mathbf{k}} \rho_{\mathbf{l}} \rho_{-\mathbf{k}-\mathbf{l}} \rangle \\ & + \frac{1}{2\Omega} \sum_{\mathbf{k} \neq 0} v_{\mathbf{k}} (\langle \rho_{\mathbf{k}} \rho_{-\mathbf{k}} \rangle - N), \end{aligned} \quad (12)$$

where $v_{\mathbf{k}} = 4\pi e^2/k^2$ and ϵ_i denotes the single particle energy given by

$$\hbar \varphi_i(\mathbf{r}) = \epsilon_i \varphi_i(\mathbf{r}). \quad (13)$$

Clearly, we need the matrix elements

$$I_2(\mathbf{k}_1, \mathbf{k}_2) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rangle, \quad (14)$$

and

$$I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \rho_{\mathbf{k}_3} \rangle, \quad (15)$$

for use in the energy formulas.

These matrix elements are many-body integrals. From classical statistical mechanics one learns how they might be evaluated with cluster expansion procedures or stochastic methods. Yet, to our taste, integral equation techniques appear more efficient and reliable. By generalizing the formalism developed in Ref. 4, we define

$$I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) \equiv \langle \rho_{\mathbf{k}_1} \rho_{\mathbf{k}_2} \cdots \rho_{\mathbf{k}_n} \rangle_{\mu}, \quad (16)$$

where the expectation value is now taken with respect to the wavefunction

$$\psi_{\mu} = D \cdot \left\{ \exp \sum_{i < j}^N \frac{\mu}{2} u(r_{ij}) \right\}. \quad (17)$$

Differentiating Eq. (16) with respect to μ , we find the recurrence relation

$$\begin{aligned} \frac{d}{d\mu} I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) \\ = \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_{n+2}(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n, \mathbf{k}, -\mathbf{k} | \mu) \\ - I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)], \end{aligned} \quad (18)$$

thus a hierarchy of differential equations. By truncating the hierarchy with a reasonable closure approximation, one can in principle solve the equations and obtain all $I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu)$, and in particular all

$$I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n) \equiv I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu = 1). \quad (19)$$

In the lowest orders, Eq. (18) yields

$$\begin{aligned} \frac{d}{d\mu} I_1(\mathbf{k}_1 | \mu) &= \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_3(\mathbf{k}_1, \mathbf{k}, -\mathbf{k} | \mu) \\ &\quad - I_1(\mathbf{k}_1 | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)] \\ \frac{d}{d\mu} I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu) &= \frac{1}{2\Omega} \sum_{\mathbf{k}} u(k) [I_4(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}, -\mathbf{k} | \mu) \end{aligned}$$

$$- I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu) I_2(\mathbf{k}, -\mathbf{k} | \mu)]. \quad (20)$$

If I_3 and I_4 are expressed in terms of I_1 and I_2 , then Eq. (20) is a set of two coupled differential equations and can be solved for $I_1(\mathbf{k} | \mu)$ and $I_2(\mathbf{k}_1, \mathbf{k}_2 | \mu)$.

In this paper, we derive general formulas for the matrix elements $I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n | \mu)$ which, in the convolution approximation are given in terms of I_1 and I_2 . Specific expressions for I_2 , I_3 , and I_4 are given. Except where noted, the model in mind will be the inhomogeneous electron liquid as defined in this section. Detailed application and results will be presented elsewhere.

II. MATHEMATICAL FORMULATION

Consider an N -particle system which possesses a nonuniform density distribution. The inhomogeneity may be the consequence of an external periodic potential such as in the case of electron liquids in solids. It may also be caused by the existence of a surface, or the presence of local impurities. We shall first formulate our analysis generally without specifying the type of inhomogeneity to encompass all these possibilities. The result will then be specialized to the case of a periodic inhomogeneity.

As mentioned in the Introduction, we wish to evaluate the multiple density correlation function

$$I_n(\mathbf{k}_1, \dots, \mathbf{k}_n | \mu) = \langle \rho_{\mathbf{k}_1} \cdots \rho_{\mathbf{k}_n} \rangle_{\mu}, \quad (21)$$

where $\langle \rangle_{\mu}$ denotes the quantum mechanical expectation value defined in Eq. (11) by the wavefunction $\psi_{\mu}(\mathbf{r}_1, \dots, \mathbf{r}_N)$ of the N -particle system. For convenience, we shall omit the subscript μ as well as all references to spins in the following.

The formal evaluation of I_n follows closely that for a homogeneous system.⁵ First, we define the n -particle distribution function

$$\begin{aligned} p_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \\ = \frac{N!}{(N-n)!} \int |\psi|^2 d\mathbf{r}_{n+1} \cdots d\mathbf{r}_N / \int |\psi|^2 d\mathbf{r}_1 \cdots d\mathbf{r}_N, \end{aligned} \quad (22)$$

which, by definition, is symmetric in its n coordinates. For a homogeneous system the one-particle distribution function $p_1(\mathbf{r})$ is a constant equal to the mean particle density $\rho = N/\Omega$. For an inhomogeneous system $p_1(\mathbf{r})$ will be dependent on spatial coordinates. Next we define the cluster functions f_2, f_3, \dots , as follows:

$$\begin{aligned} p_2(\mathbf{r}_1, \mathbf{r}_2) &= p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) [1 + f_2(\mathbf{r}_1, \mathbf{r}_2)], \\ p_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) &= p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) [1 + f_2(\mathbf{r}_1, \mathbf{r}_2) + f_2(\mathbf{r}_2, \mathbf{r}_3) \\ &\quad + f_2(\mathbf{r}_3, \mathbf{r}_1) + f_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)], \end{aligned} \quad (23)$$

etc.

Further, define the Fourier transforms:

$$\pi(\mathbf{k}) = \int p_1(\mathbf{r}) \exp(i\mathbf{k} \cdot \mathbf{r}) d\mathbf{r}, \quad (24)$$

$$p_1(\mathbf{r}) = \frac{1}{\Omega} \sum_{\mathbf{k}} \pi(\mathbf{k}) \exp(-i\mathbf{k} \cdot \mathbf{r}), \quad (25)$$

$$F_n(\mathbf{k}_1, \dots, \mathbf{k}_n)$$

$$= \int p_1(\mathbf{r}_1) \dots p_1(\mathbf{r}_n) f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_n \cdot \mathbf{r}_n)] d\mathbf{r}_1 \dots d\mathbf{r}_n, \quad n \geq 2. \quad (26)$$

It is then a direct consequence of these definitions that the expectation value (21) can be written as⁵

$$I_1(\mathbf{k}) = \pi(\mathbf{k}),$$

$$I_2(\mathbf{k}_1, \mathbf{k}_2) = \pi(\mathbf{k}_1)\pi(\mathbf{k}_2) + U_2(\mathbf{k}_1, \mathbf{k}_2), \quad (27)$$

$$I_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \pi(\mathbf{k}_1)\pi(\mathbf{k}_2)\pi(\mathbf{k}_3) + \pi(\mathbf{k}_1)U_2(\mathbf{k}_2, \mathbf{k}_3) + \pi(\mathbf{k}_2)U_2(\mathbf{k}_3, \mathbf{k}_1) + \pi(\mathbf{k}_3)U_2(\mathbf{k}_1, \mathbf{k}_2) + U_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3),$$

etc.,

where

$$U_2(\mathbf{k}_1, \mathbf{k}_2) = \pi(\mathbf{k}_1 + \mathbf{k}_2) + F_2(\mathbf{k}_1, \mathbf{k}_2),$$

$$U_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) = \pi(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) + F_2(\mathbf{k}_1, \mathbf{k}_2 + \mathbf{k}_3) + F_2(\mathbf{k}_2, \mathbf{k}_3 + \mathbf{k}_1) + F_2(\mathbf{k}_3, \mathbf{k}_1 + \mathbf{k}_2) + F_3(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3), \quad (28)$$

etc.

This completes the formal evaluation of I_n . While Eqs. (27) and (28) are exact, the usefulness of this formulation rests in the fact that $U_n(\mathbf{k}_1, \dots, \mathbf{k}_n)$ assumes a simple form when the convolution approximation is used for p_n . This will then make the evaluation of I_n practical for reasonably large values of n . The rest of this paper will be devoted to evaluating U_n . However, there also exist some general properties of the F and U functions which are exact. We now describe these properties.

An immediate consequence of the definition (22) of p_n is the sequential relation⁵

$$\int p_1(\mathbf{r}) d\mathbf{r} = N, \quad (29)$$

$$\int p_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = (N-n)p_n(\mathbf{r}_1, \dots, \mathbf{r}_n), \quad n \geq 1. \quad (30)$$

Equations (29) and (30) imply, in turn, the following conditions on f_n :

$$\int p_1(\mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) d\mathbf{r}_2 = -1, \quad (31)$$

$$\int p_1(\mathbf{r}_{n+1}) f_{n+1}(\mathbf{r}_1, \dots, \mathbf{r}_{n+1}) d\mathbf{r}_{n+1} = -n f_n(\mathbf{r}_1, \dots, \mathbf{r}_n), \quad n \geq 2. \quad (32)$$

Note that Eq. (31), which reflects the normalization of f_2 , is a rather stringent condition. It will play an essential role in later discussions.

In terms of the F functions, conditions (31) and (32) lead to

$$F_2(\mathbf{k}_1, 0) = -\pi(\mathbf{k}_1), \quad (33)$$

$$F_{n+1}(\mathbf{k}_1, \dots, \mathbf{k}_n, 0) = -n F_n(\mathbf{k}_1, \dots, \mathbf{k}_n). \quad (34)$$

It then follows from Eq. (28) that

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = 0 \text{ for any } k_i = 0, \quad n \geq 2. \quad (35)$$

Equation (35) is an exact result, and is a direct consequence of the sequential relation. Assuming reasonable behavior for U_n , we then expect U_n to go to zero smoothly for small k_i . In fact, we shall explicitly see that under the convolution approximation of p_n which preserves the sequential relation, U_n vanishes linearly in k_i . However, it must be pointed out that it is not generally true that U_n is continuous at $k_i = 0$ such as in

the case of a short-range Jastrow function with $D = 1$. For such systems U_n will not vanish in the $k_i \rightarrow 0$ limit.

Another consequence of the definitions is that the function U_n is of the order of N .⁵ This is so because the moving of one particle to infinity reduces the n -particle distribution function to $(n-1)$ -particle distribution function. As a consequence, we expect

$$\lim_{r_i \rightarrow \infty} f_n(\mathbf{r}_1, \dots, \mathbf{r}_n) = 0, \quad 1 \leq i < j \leq n. \quad (36)$$

The assertion then follows from Eqs. (28) and (26). Similarly we expect $\pi(\mathbf{k})$ to be of the order of N if it does not vanish.

It proves convenient to introduce the Fourier transforms

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = \frac{1}{\Omega^2} \int f_2(\mathbf{r}_1, \mathbf{r}_2) \exp[-i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2,$$

or

$$f_2(\mathbf{r}_1, \mathbf{r}_2) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \theta(\mathbf{K}_1, \mathbf{K}_2) \exp[i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)]. \quad (37)$$

It is easily verified that the normalization condition (31) of f_2 can be written as

$$\sum_{\mathbf{K}_2} \pi(\mathbf{K}_2) \theta(\mathbf{K}_1, \mathbf{K}_2) = -\delta_{\mathbf{K}_1}(\mathbf{K}_1, 0), \quad (38)$$

where $\delta_{\mathbf{K}_1}$ is the Kronecker delta function. The following identities implied by Eq. (38) will be used in later discussions:

$$\pi(\mathbf{k}) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{K}_1) \pi(\mathbf{k} + \mathbf{K}_2) [-\theta(\mathbf{K}_1 - \mathbf{k}, \mathbf{K}_2 + \mathbf{k})], \quad (39)$$

$$\pi(\mathbf{k}_1 + \mathbf{k}_2) = \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2) [-\theta(\mathbf{K}_1 - \mathbf{k}_2, \mathbf{K}_2 + \mathbf{k}_2)]. \quad (40)$$

Despite its apparent asymmetric appearance, Eq. (40) is actually symmetric in \mathbf{k}_1 and \mathbf{k}_2 .

III. CONVOLUTION APPROXIMATION

In the development of the theory of liquid ⁴He, Jackson and Feenberg⁶ proposed a convolution approximation for the three-particle distribution function, p_3 , which satisfies the sequential relation exactly. The convolution form has since been extended to p_n for general n ,⁷ and used in the evaluation of I_n for a homogeneous system.⁵ To evaluate I_n for inhomogeneous systems, we shall therefore first need a generalization of the convolution approximation.

It is straightforward to generalize the convolution form for p_3 . Using Eq. (31), one easily verifies that the expression

$$p_3^{(c)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) [1 + f_{12} + f_{23} + f_{31} + f_{12} f_{23} + f_{23} f_{31} + f_{31} f_{12} + \int p_1(\mathbf{r}_4) f_{14} f_{24} f_{34} d\mathbf{r}_4] \quad (41)$$

satisfies the sequential relation Eq. (30) for $n = 2$.

Here, we have adopted the shorthand notation

$$f_{ij} = f_2(\mathbf{r}_i, \mathbf{r}_j).$$

Since Eq. (41) reduces to the convolution form for p_3

$$p_3^{(c)} = 1 + \begin{array}{c} 1 \\ \circ \\ 2 \end{array} + \begin{array}{c} 2 \\ \circ \\ 3 \end{array} + \begin{array}{c} 3 \\ \circ \\ 1 \end{array} + f_3^{(c)}$$

$$f_3^{(c)} = \begin{array}{c} 2 \\ \circ \\ 1 \end{array} + \begin{array}{c} 3 \\ \circ \\ 2 \end{array} + \begin{array}{c} 1 \\ \circ \\ 3 \end{array} + \begin{array}{c} 1 \\ \circ \\ 2 \end{array}$$

FIG. 1. Graphical representation of $p_3^{(c)}$.

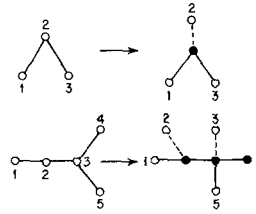


FIG. 3. Examples of graph normalization.

of Refs. 6 and 7 upon taking $p_1(\mathbf{r}) = \rho$, it is a natural generalization of the convolution approximation.

To further generalize Eq. (41) to $p_n^{(c)}$ for $n > 3$, it is convenient, as in Ref. 7, to use graphical terms for algebraic expressions.

We refer to Ref. 7 for definitions of terms in linear graph theory. It is seen that Eq. (41) can be represented by precisely the same graphs as in Ref. 7, which we reproduce in Fig. 1. However, the following rules will now be used to convert graphs into algebraic expressions:

- (i) The line joining two root points labeled i and j carries a weight f_{ij} .
- (ii) The root point labeled i carries a weight $p_1(\mathbf{r}_i)$.
- (iii) Each black point carries a dummy label k and a weight

$$\int p_1(\mathbf{r}_k) d\mathbf{r}_k.$$

- (iv) The algebraic expression represented by a graph is the product of the weights in (i)–(iii).

With the diagram rules (i)–(iv), it is not difficult to see that the analysis of Ref. 7 can be carried through without change. The key step is, of course, the utilization of the normalization condition (31). The consideration eventually leads to the same expression of $p_n^{(c)}$ as in Ref. 7.

For our purpose, it suffices to give only the expression for f_n . One finds as in Ref. 7

$$[\prod_i p_i(\mathbf{r}_i)] f_n^{(c)}(\mathbf{r}_1, \dots, \mathbf{r}_n) \quad (42)$$

= the collection of all distinct, connected, n -rooted Cayley trees, provided that all black points are nodes.

As an example, $f_3^{(c)}$ is shown in Fig. 1.

We now substitute Eq. (42) into Eq. (26) to evaluate $F_n^{(c)}$, the convolution form for F_n . The result is most conveniently expressed in terms of the Fourier transformed functions $\pi(\mathbf{k})$ and $\theta(\mathbf{K}_1, \mathbf{K}_2)$. The substitution leads to

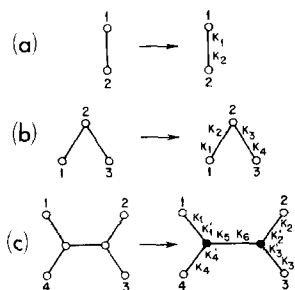


FIG. 2. Graphical representations of expressions (45)–(47).

$$F_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) = \text{the same graphs as in Eq. (42),} \quad (43)$$

provided that the following graph rules are used:

- (a) Cut each line into two halves at the midpoint and label the two halves with momenta \mathbf{K}_α and \mathbf{K}_β respectively.

- (b) The line labeled \mathbf{K}_α and \mathbf{K}_β carries a weight

$$\sum_{\mathbf{K}_\alpha, \mathbf{K}_\beta} \theta(\mathbf{K}_\alpha, \mathbf{K}_\beta). \quad (44)$$

- (c) The root point labeled i carries a weight $\pi(\mathbf{k}_i + \sum \mathbf{K}_\alpha)$, where $\sum \mathbf{K}_\alpha$ is the sum of the momenta of the half-lines incident at the root point.

- (d) Each black point carries a weight $\pi(\sum \mathbf{K}_\alpha)$, where $\sum \mathbf{K}_\alpha$ has the same meaning as in (c).

- (e) The algebraic expression of a graph in Eq. (43) is the product of all the weights in (b)–(d).

Note that we have numbered the momentum-space graph rules by Roman letters to distinguish them from the rules in the \mathbf{r} -space. Some typical terms in Eq. (43) are shown in Fig. 2 with the algebraic expressions given as follows:

$$\begin{aligned} \text{(a)} \quad & F_2(\mathbf{k}_1, \mathbf{k}_2) \\ &= \int p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) f_2(\mathbf{r}_1, \mathbf{r}_2) \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2 \\ &= \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2) \theta(\mathbf{K}_1, \mathbf{K}_2), \end{aligned} \quad (45)$$

$$\begin{aligned} \text{(b)} \quad & \int p_1(\mathbf{r}_1) p_1(\mathbf{r}_2) p_1(\mathbf{r}_3) f_{12} f_{23} \\ & \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \mathbf{k}_2 \cdot \mathbf{r}_2 + \mathbf{k}_3 \cdot \mathbf{r}_3)] d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_3 \\ &= \sum_{\mathbf{K}_1, \dots, \mathbf{K}_4} \pi(\mathbf{k}_1 + \mathbf{K}_1) \pi(\mathbf{k}_2 + \mathbf{K}_2 + \mathbf{K}_3) \pi(\mathbf{k}_3 + \mathbf{K}_4) \\ & \times \theta(\mathbf{K}_1, \mathbf{K}_2) \theta(\mathbf{K}_3, \mathbf{K}_4), \end{aligned} \quad (46)$$

$$\begin{aligned} \text{(c)} \quad & \int p_1(\mathbf{r}_1) \dots p_6(\mathbf{r}_6) f_{15} f_{45} f_{26} f_{36} f_{56} \\ & \times \exp[i(\mathbf{k}_1 \cdot \mathbf{r}_1 + \dots + \mathbf{k}_6 \cdot \mathbf{r}_6)] d\mathbf{r}_1 \dots d\mathbf{r}_6 \\ &= \sum_{\mathbf{K}_i} \sum_{\mathbf{K}'_i} \left[\prod_{i=1}^4 \pi(\mathbf{k}_i + \mathbf{K}_i) \theta(\mathbf{K}_i, \mathbf{K}'_i) \right] \theta(\mathbf{K}_5, \mathbf{K}_6) \\ & \times \pi(\mathbf{K}'_1 + \mathbf{K}'_4 + \mathbf{K}_5) \pi(\mathbf{K}'_2 + \mathbf{K}'_3 + \mathbf{K}_6). \end{aligned} \quad (47)$$

We are now in a position to evaluate $U_n^{(c)}$ by combining Eqs. (43) and (28). To this end it is convenient to introduce the normal graphs as in Ref. 5. Whenever a rooted point, labeled i , say, occurs as an interior point, the graph is "normalized" by converting the root point into a black point, adding a new root point with the same label i , and connecting the new root point to

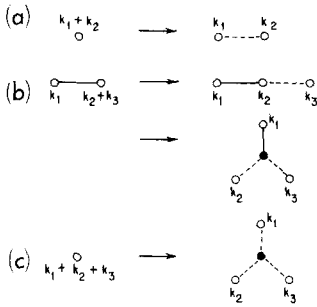


FIG. 4. Examples of graph normalization where the momentum label is the sum of individual momenta.

the black point by a broken line. Some examples of this normalization procedure are shown in Fig. 3. Although a new (broken) line and a new point are added to the graph, the graph weight can be made unchanged if we use identity (39), and associate with a broken line the weight

$$-\sum_{\mathbf{K}_1, \mathbf{K}_2} \theta(\mathbf{K}_1 - \mathbf{k}_i, \mathbf{K}_2 + \mathbf{k}_i). \quad (48)$$

Here the diagram rules (a)–(e) are followed except that the weight (48) is used in place of (44) for broken lines. In (48), \mathbf{K}_2 is the momentum label of the half-dashed line incident to the new root point.

The above normalization procedure can be applied in succession to graphs whose labels are sums of individual momenta. Some examples are shown in Fig. 4. Here, Fig. 4(a) is precisely the graphical representation of identity (40); Fig. 4(c) reads

$$\begin{aligned} & \pi(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) \\ &= \sum_{\mathbf{K}_1, \mathbf{K}'_i} \left\{ \prod_{i=1}^3 \pi(\mathbf{k}_i + \mathbf{K}_i) [-\theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \right\} \\ & \quad \times \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3). \end{aligned} \quad (49)$$

An expression for Fig. 4(b) can be similarly obtained from the graph using the rules (a)–(e).

After all graphs in Eq. (43) are normalized, we arrive at

$$\begin{aligned} & U_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \\ &= \text{the collection of all distinct normal } n\text{-rooted} \\ & \text{Cayley trees whose black points are nodes. The terminal} \\ & \text{lines are either solid or broken.} \end{aligned} \quad (50)$$

(Terminal lines are the lines incident to the root points which are now on the surface of the Cayley tree.) Now, each terminal line is either solid or broken, irrespective of the condition on other lines; we may therefore combine the solid and broken lines to form a double terminal line and obtain

$$\begin{aligned} & U_n^{(c)}(\mathbf{k}_1, \dots, \mathbf{k}_n) \\ &= \text{the collection of all distinct normal } n\text{-rooted} \\ & \text{Cayley trees whose black points are nodes and whose} \\ & \text{terminal lines are double lines.} \end{aligned} \quad (51)$$

The double (terminal) line now carries a weight which is given by combining Eq. (44) and (48),

$$\sum_{\mathbf{K}_1, \mathbf{K}_2} [\theta(\mathbf{K}_1, \mathbf{K}_2) - \theta(\mathbf{K}_1 - \mathbf{k}_i, \mathbf{K}_2 + \mathbf{k}_i)]. \quad (52)$$

Here, as in Eq. (48), \mathbf{K}_2 is the momentum of the half-double line incident to the root point labeled i .

Equation (51) is identical to the result of Ref. 5,

except that the graph rules are now (a)–(e) with Eq. (52) in place of Eq. (44) for terminal lines. Graphs for $U_n^{(c)}$ have been given in Fig. 5 of Ref. 5 for $n \leq 5$. We give here only the explicit expression for $n = 2, 3, 4$:

$$\begin{aligned} U_2(\mathbf{k}_1, \mathbf{k}_2) &= \sum_{\mathbf{K}_1, \mathbf{K}_2} \pi(\mathbf{K}_1 + \mathbf{k}_1) \pi(\mathbf{K}_2 + \mathbf{k}_2) \\ & \quad \times [\theta(\mathbf{K}_1, \mathbf{K}_2) - \theta(\mathbf{K}_1 - \mathbf{k}_2, \mathbf{K}_2 + \mathbf{k}_2)], \end{aligned} \quad (53)$$

$$\begin{aligned} U_3^{(c)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3) &= \sum_{\mathbf{K}_i, \mathbf{K}'_i} \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3) \prod_{i=1}^3 \{ \pi(\mathbf{K}_i + \mathbf{k}_i) \\ & \quad \times [\theta(\mathbf{K}'_i, \mathbf{K}_i) - \theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \}, \end{aligned} \quad (54)$$

$$\begin{aligned} & U_4^{(c)}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4) \\ &= \sum_{\mathbf{K}_i, \mathbf{K}'_i} \prod_{i=1}^4 \{ \pi(\mathbf{K}_i + \mathbf{k}_i) [\theta(\mathbf{K}'_i, \mathbf{K}_i) \\ & \quad - \theta(\mathbf{K}'_i - \mathbf{k}_i, \mathbf{K}_i + \mathbf{k}_i)] \} [\pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}'_3 + \mathbf{K}'_4) \\ & \quad + \pi(\mathbf{K}'_1 + \mathbf{K}'_2 + \mathbf{K}_5) \pi(\mathbf{K}'_3 + \mathbf{K}'_4 + \mathbf{K}_6) \theta(\mathbf{K}_5, \mathbf{K}_6)]. \end{aligned} \quad (55)$$

Note that Eq. (52) implies $U_n^{(c)} \sim k_i$ for any $k_i \sim 0$ if the function θ has a Taylor's expansion. This is the result alluded to earlier in the text.

IV. APPLICATIONS

The expression (51) for U_n has been derived using the convolution approximation; otherwise it is an exact result. In applications further simplification usually arises either due to some special properties of the physical system or additional approximations introduced for convenience. To make our formulation useful we now describe some of these simplifications.

Consider first the case of a homogeneous system. For an isotropic and homogeneous many-particle system we expect $\rho_1(\mathbf{r}) = \rho$ and the two-particle distribution function $\rho_2(\mathbf{r}_1, \mathbf{r}_2)$ to depend only on the distance between the two particles, or

$$f_2(\mathbf{r}_1, \mathbf{r}_2) = h(r_{12}). \quad (56)$$

Thus from Eq. (37) we find

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = N^{-1} u(K_1) \delta_{\mathbf{K}\mathbf{r}}(\mathbf{K}_1 + \mathbf{K}_2, 0), \quad (57)$$

where

$$u(k) = \rho \int \exp(i\mathbf{k} \cdot \mathbf{r}) h(r) d\mathbf{r}. \quad (58)$$

The normalization condition now reads

$$u(0) = -1. \quad (59)$$

Also from Eq. (25),

$$\pi(\mathbf{k}) = N \delta_{\mathbf{K}\mathbf{r}}(\mathbf{k}, 0). \quad (60)$$

Substituting these results into Eq. (51), we see that the graph rules (a)–(e) may be greatly simplified. In particular, each line now carries a single momentum label and a weight $u(\mathbf{K})$ for internal lines and weight $u(k_i) - u(0)$ for terminal lines. The root and black points carry no weight except that momentum is conserved at black points. This is the result of Ref. 7.

In the application to inhomogeneous systems it may be necessary for reasons of practicality to assume approximation (56), even though the one-particle distribution function should still be dependent on spatial

coordinates. Again, this leads to a single momentum label for each line and the graph rules are simplified accordingly.

Finally, we consider the application to a system with periodic inhomogeneity. For such a system the n -particle distribution function (23) is expected to remain unchanged under the translation \mathbf{R} of *all* particle coordinates, where \mathbf{R} is any lattice vector of the underlying Bravais lattice.⁸ This says in particular

$$p_1(\mathbf{r} + \mathbf{R}) = p_1(\mathbf{r}) \quad (61)$$

and

$$f_n(\mathbf{r}_1 + \mathbf{R}, \dots, \mathbf{r}_n + \mathbf{R}) = f_n(\mathbf{r}_1, \dots, \mathbf{r}_n). \quad (62)$$

It then follows from Eqs. (25) and (37) that

$$\pi(\mathbf{k}) = M \delta_{\mathbf{k}\mathbf{r}}(\mathbf{k}, \mathbf{G}) \tau(\mathbf{G}) \quad (63)$$

and

$$\theta(\mathbf{K}_1, \mathbf{K}_2) = M \delta_{\mathbf{K}\mathbf{r}}(\mathbf{K}_1 + \mathbf{K}_2, \mathbf{G}) \sigma(\mathbf{K}_1, \mathbf{K}_2), \quad (64)$$

where

$$\tau(\mathbf{G}) = \int_{\text{unit cell}} d\mathbf{r} p_1(\mathbf{r}) \exp(i\mathbf{G} \cdot \mathbf{r}), \quad (65)$$

and

$$\begin{aligned} \sigma(\mathbf{K}_1, \mathbf{K}_2) = & \int_{\text{unit cell}} d\mathbf{r}_1 \int d\mathbf{r}_2 f_2(\mathbf{r}_1, \mathbf{r}_2) \\ & \times \exp[-i(\mathbf{K}_1 \cdot \mathbf{r}_1 + \mathbf{K}_2 \cdot \mathbf{r}_2)]. \end{aligned} \quad (66)$$

In Eqs. (63) and (64), M is the number of unit cells of the periodic lattice, and \mathbf{G} is a reciprocal lattice vector satisfying

$$\exp(i\mathbf{G} \cdot \mathbf{R}) = 1. \quad (67)$$

Similarly, Eqs. (62), (26), and (28) imply that

$$U_n(\mathbf{k}_1, \dots, \mathbf{k}_n) = M \delta_{\mathbf{K}\mathbf{r}}(\mathbf{k}_1 + \dots + \mathbf{k}_n, \mathbf{G}) u_n, \quad n \geq 2, \quad (68)$$

where $u_n = O(1)$. Note that Eq. (68) is an exact result valid for any system satisfying Eq. (62).

V. CONCLUSION

We have evaluated in a closed form the multiple density correlation function I_n for a nonuniform system. The exact expression of I_n is given in Eqs. (27) and (28) in terms of the cluster integrals U_n . In Sec. III we generalized the convolution approximation for the n -particle distribution function to nonuniform systems, and used this approximation to evaluate U_n . This leads to the closed form expression (51) for U_n . Explicit expressions for $n=2, 3, 4$ are given in (53)–(55). Finally in Sec. V the formulation is specialized to specific systems including the case of a periodic inhomogeneity.

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⁸Equation (61) may be proved rigorously for a many-particle system in an external periodic potential. Let $T_{\mathbf{R}}$ be a translation operator which displaces *all* particle coordinates by \mathbf{R} . Since $T_{\mathbf{R}}$ commutes with the Hamiltonian, H , the wavefunction ψ can be chosen to be the simultaneous eigenfunction of $T_{\mathbf{R}}$ and H . Further, since $T_{\mathbf{R}} T_{\mathbf{R}'} = T_{\mathbf{R}+\mathbf{R}'}$, the eigenvalues of $T_{\mathbf{R}}$ are necessarily of the form $e^{i\mathbf{k}\cdot\mathbf{R}}$, or $T_{\mathbf{R}}\psi = e^{i\mathbf{k}\cdot\mathbf{R}}\psi$. The numbers \mathbf{k} are determined by the usual Born-von Karman boundary condition and are real. It follows then that $|T_{\mathbf{R}}\psi|^2 = |\psi|^2$ and, consequently, $T_{\mathbf{R}}p_n = p_n$.

Scaling invariance of helical curve motion and soliton equations^{a)}

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The scaling properties of the equations describing the motion of helical curves determine the scaling of the associated nonlinear evolution equations. Only two polynomial scaling-invariant evolution equations can be found. Of these, the nonlinear Schrödinger equation has the physically correct scaling invariance, but the modified Korteweg–de Vries can not be connected to realistic helical curves.

Many physical phenomena and the equations that describe them are invariant under a change in scale. Scaling invariance of a linear equation leaves the dependent variable unaffected, but in nonlinear equations the dependent variable must typically scale in some specific way to retain the invariance, depending on the equation.

In an extension of Hasimoto's work,¹ Lamb² recently found an interesting connection between various nonlinear evolution equations and the motion of vortex filaments or helical curves. The vortex motion equations are linear, and yield in a natural way the linear inverse scattering equations associated with the nonlinear evolution equations. The equations in question are the sine–Gordon and Hirota³ equations. The latter contains the modified Korteweg–de Vries and nonlinear Schrödinger equation as special cases.

This paper shows that scaling invariance⁴ of the vortex equations (1) is consistent only with one particular scaling of the nonlinear evolution equation, namely that of the nonlinear Schrödinger equation. Specifically, only this equation is connected to physically realizable vortex motion, i. e., motion with a given scaling invariant circulation. The other evolution equations discussed by Lamb can be obtained by allowing the circulation to change with scaling, or by considering a different dependent variable.

It is worth noting that invariance transformations of nonlinear evolution equations have been investigated recently in some detail.⁵ That work exploited group-theoretical properties of infinitesimal invariance transformations. The scaling transformation used here is finite, and can be generated by iteration of its infinitesimal counterpart. We consider the finite scaling transformation because it is a fairly obvious and convenient, but yet nontrivial and hence an attractive means for a preliminary investigation of nonlinear equations. For completeness we note that nonlinear equations with soliton behavior need not be scaling invariant.^{3,4}

The association of nonlinear equations with helical motion proceeds as follows.^{1,2}

The Serret–Frenet equations are

$$\hat{t}_s = \kappa \hat{n}, \tag{1a}$$

$$\hat{b}_s = -\tau \hat{n} \tag{1b}$$

$$\hat{n}_s = \tau \hat{b} - \kappa \hat{t}, \tag{1c}$$

where the subscript denotes partial differentiation with respect to the arc length s and the functions $\kappa(s, t)$ and $\tau(s, t)$ are curvature and torsion respectively, which also depend on the time t . The tangent vector \hat{t} is defined by the derivative of the position vector $X(s, t)$,

$$\hat{t} \equiv X_s(s, t), \tag{1d}$$

while \hat{n} and \hat{b} are the normal and binormal to the curve.

The motion of the vortex is approximated by

$$X_t = G \kappa \hat{b}, \tag{1e}$$

where G is proportional to the circulation, the integral of fluid velocity around the vortex. The vortex strength G is constant for any one vortex, and can be chosen unity by suitable normalization of time t .

With introduction of the complex vector $N(s, t)$,

$$N \equiv (\hat{n} + i\hat{b}) \exp[i \int_{-\infty}^s ds' (\tau - \tau_0)], \tag{2a}$$

and the complex scalar

$$\psi \equiv \kappa \exp[i \int_{-\infty}^s ds' (\tau - \tau_0)], \tag{2b}$$

(τ_0 is the asymptotic value of the torsion as $|s| \rightarrow \infty$), combination of Eqs. (1a)–(1c) yields

$$N_s + i\tau_0 N = -\psi \hat{t}, \tag{3a}$$

$$\hat{t}_s = \frac{1}{2}(\psi^* N + \psi N^*). \tag{3b}$$

The function ψ will be the dependent variable in the nonlinear evolution equation, and is assumed to vanish as $|s| \rightarrow \infty$.

The norm-preserving variation of N and \hat{t} in time, on the other hand, can be written as¹

$$N_t = iRN + \gamma \hat{t}, \tag{4a}$$

$$\hat{t}_t = -\frac{1}{2}(\gamma^* N + \gamma N^*), \tag{4b}$$

where $R(s, t)$ is real and $\gamma(s, t)$ complex. The equation of motion (1e) can be expressed as

$$X_t \equiv C^* \psi^* N + C \psi N^* + \theta \hat{t}, \quad C \equiv \frac{1}{2}(\zeta + i\eta), \tag{4c}$$

where ζ, η , and θ are real functions of s and t yet to be determined. Equating mixed second derivatives of

^{a)}Work done under the auspices of the U.S. Energy Research and Development Administration.

N from (3) and (4) yields

$$\psi_t + \gamma_s + i(\tau_0 \gamma - R\psi) = 0, \quad (5a)$$

$$R_s = \frac{1}{2}i(\gamma\psi^* - \gamma^*\psi). \quad (5b)$$

Furthermore, use of $X_{st} = X_{ts}$ gives²

$$-\frac{1}{2}\gamma = (C\psi)_s + i\tau_0 C\psi + \frac{1}{2}\theta\psi, \quad (6a)$$

$$\theta_s = \zeta |\psi|^2, \quad (6b)$$

and, using Eq. (2b),

$$R_s = (\eta |\psi|^2)_s - \frac{1}{2}\eta |\psi|^2_s - \theta_s \tau. \quad (6c)$$

The desired evolution equation for ψ , Eq. (5a), contains only one time derivative. The auxiliary functions R, γ, ζ , and θ are related by Eqs. (5b)–(6c). The linear inverse scattering equations, which allow us to solve Eq. (5a) for ψ analytically, follow from (3) and (6) as shown by Lamb. They contain R and γ with τ_0 as the eigenvalue.

How do Eqs. (1)–(6) behave under a scaling transformation of the spatial coordinate s and time t ? This transformation has the form

$$s' = \alpha s, \quad (7a)$$

$$t' = \alpha^h t. \quad (7b)$$

The scaling variable α and exponent h are real.

We first consider scaling of the spatial coordinate s . The spatial position X should transform like s , Eq. (7a). Thus the tangent vector \hat{t} , Eq. (1d), is invariant, consistent with the physical meaning of \hat{t} as the unit vector tangent to curve $X(s)$. The scaling of curvature $\kappa(s, t)$, torsion $\tau(s, t)$, and thus the dependent variable ψ is, from Eqs. (1a)–(1c), given by

$$\psi(s, t) = \alpha \psi'(s', t'). \quad (7c)$$

The phase of ψ ,

$$\sigma(s, \tau) \equiv \int_{-\infty}^s ds' (\tau - \tau_0), \quad (7d)$$

is invariant: Only the magnitude of ψ changes under scaling. The unit vector \hat{n} , \hat{b} , and thus N , are invariant as they should.

At this point we can already negate a direct association between helical curve motion and those nonlinear evolution equations with a scaling different from Eq. (7c). An example is: the Korteweg–de Vries equation $\phi_t + \phi\phi_s + \phi_{sss} = 0$. Comparing the terms $\phi\phi_s$ and ϕ_{sss} it is clear that ϕ scales according to $\phi(s) = \alpha^2 \phi'(s')$, in contrast to Eq. (7c). Thus the Korteweg–de Vries equation can not be identified with the evolution equation (5). [We refrain from additional transformations on the dependent variables, such as the Miura transformation,⁶ which connects the KdV equation to the modified KdV equation: The MKdV equation, with nonlinear term $\phi^2 \phi_s$, has the correct scaling (7c).]

Having studied the scaling properties of the purely geometrical part of helical curve motion, we now proceed to examine scaling of time according to Eq. (7b) in the equation of motion (1e). The parameter G , proportional to an integral of velocity \times length, scales as $G = \alpha^{2-h} G$. When in addition we use the scaling of κ , we see that Eq. (1e) is only scaling invariant when $h = 2$.

Hasimoto¹ found the corresponding nonlinear Schrödinger equation, which is the only possible one as will become clear later.

However, we could artificially consider a vortex with circulation G dependent on the scaling parameter α as $G(\alpha) = G(\alpha = 1)\alpha^{2h-4}$. Equivalently, we could choose Eq. (1e) for our dynamical equation, but refrain from an interpretation in terms of vortices. Then nothing compels us to take $h = 2$, and we can consider h an arbitrary real constant.

With this assumption it follows from the defining relations (4) that the auxiliary functions R and γ , η and ζ , and θ scale as

$$R(s, t) = \alpha^h R'(s', t'), \quad \gamma(s, t) = \alpha^h \gamma'(s', t'), \quad (8a)$$

$$\eta(s, t) = \alpha^{h-2} \eta'(s', t'), \quad \zeta(s, t) = \alpha^{h-2} \zeta'(s', t'), \quad (8b)$$

$$\theta(s, t) = \alpha^{h-1} \theta'(s', t'). \quad (8c)$$

The desired evolution equation (5a) is also scaling invariant, since it follows from scaling-invariant equations (1) and (4).

At this point Eq. (5a) is an evolution equation for ψ with unknown functions $R(s, t)$ and $\gamma(s, t)$. Through Eq. (6) these functions are functionals of ψ . Equation (6) contains only multiplications of the functions R, γ, η, ζ , and θ with each other and with ψ and its s derivatives. This suggests that R, \dots, θ can be chosen as polynomials⁷ of ψ and its s derivatives, with τ_0 appearing as a parameter, and the coefficients independent of s or t . Consequently, the evolution equation is also a polynomial in these variables.

The individual terms in a scaling invariant polynomial must each scale in the same way as that polynomial. Each polynomial, R, γ , etc., occurring in Eqs. (5) and (6) can thus be written as a sum of specific terms, with coefficients that follow from (5) and (6). Below we give an example of this procedure for $h = 4$.

The choice $h = 2$ and $h = 3$ respectively yields the nonlinear Schrödinger equation $i\psi_t + 2\psi_{ss} + |\psi|^2 \psi = 0$, and the modified Korteweg–de Vries equation $\psi_t + \frac{3}{2}\psi^2 \psi + \psi_{sss} = 0$. It is clear by inspection that the scaling (7) leaves these equations invariant. Furthermore, the functions R and γ are invariant: for example, when $h = 2$ we have²

$$R = |\psi|^2 - 2\tau_0^2 \text{ and } \gamma = 2i\psi_s - 2\tau_0 \psi.$$

Restricting the functional dependence of $G(\alpha)$ to powers of the scaling factor α can only yield evolution equations that are scaling invariant. A more general functional dependence for $G(\alpha)$ allows the Hirota equation, which is not scaling invariant.

Instead of considering evolution equations with dependent variable ψ one can look for evolution equations with dependent variable the phase σ , given in Eq. (7d). This quantity is scaling invariant, just as any functional of σ . Therefore, evolution equations for σ are not restricted to polynomials, unlike evolution equations for ψ . For σ one finds the sine–Gordon equation $\sigma_{st} = \sin\sigma$. This equation also follows when one considers

$\sigma = \int_{-\infty}^s \psi(s, t) ds$. However, the scaling exponent h becomes $h = -1$, which is not physically realizable.

We now attempt to find an evolution equation for ψ with scaling exponent $h = 4$. Consider the polynomial ξ with scaling power $h - 2 = 2$. Its most general form is a sum of all possible real terms, each with scaling factor α^2 :

$$\xi = c_1 |\psi|^2 + c_2 \tau_0^2 + c_3 \tau_0 (\psi + \psi^*) + ic_4 \tau_0 (\psi - \psi^*) + c_5 (\psi_s + \psi_s^*) + ic_6 (\psi_s - \psi_s^*), \quad (9)$$

where the coefficients $c_1 - c_6$ are arbitrary real numbers, to be determined by Eqs. (6b), (6a), and (5a). (A term such as $\tau_0^{-1} \psi_{ss}$ is excluded because τ_0 must be allowed to take any real value, including zero.) Equation (6b) implies

$$\int_{-\infty}^{\infty} \xi |\psi|^2 ds = 0, \quad (10)$$

for arbitrary ψ . Thus the coefficients $c_1 - c_6$ all vanish, as none of the terms cancel, or can be integrated to zero. Consequently, $\xi = 0 = \theta$. Since $\theta_s = 0$ and the s dependence in θ enters only through $\psi(s, t)$, θ is independent of ψ , and can only be a function of the constant parameter τ_0 . Because θ scales with exponent $h - 1 = 3$ [Eq. (8c)], the most general form of θ is $\theta = a\tau_0^3$, where a is an arbitrary real constant. The functions η and R , with scaling exponents $h - 2 = 2$ and $h = 4$ respectively, follow in a similar way from Eq. (6c) as

$$\eta = b |\psi|^2 + c\tau_0^2, \quad (11a)$$

$$R = \frac{3}{4} b |\psi|^4 + \frac{1}{2} c\tau_0^2 |\psi|^2. \quad (11b)$$

Equation (6a) now yields for γ :

$$\gamma = -ib(|\psi|^2 \psi)_s - ic\tau_0^2 \psi_s + \tau_0 b |\psi|^2 \psi + (c - a)\tau_0^3 \psi. \quad (11c)$$

Substituting R and γ in Eq. (5a) leads to

$$\psi_t - ib(|\psi|^2 \psi)_{ss} - \frac{3}{4} b |\psi|^4 \psi + 2b\tau_0(|\psi|^2 \psi)_s + \tau_0^2 [-ic\psi_{ss} + (ib - \frac{1}{2}c)|\psi|^2 \psi] + (2c - a)\tau_0^3 \psi_s + i(c - a)\tau_0^4 \psi = 0. \quad (12)$$

The parameter τ_0 is the eigenvalue of the linear scattering equations,² and has to be determined by them.

Consequently, we must choose the constants a , b , and c such that τ_0 disappears from Eq. (12); hence the trivial result $a = b = c = 0$, $\psi_t = 0$.

Proceeding in a similar way the case $h = 5$ again yields the trivial equation $\psi_t = 0$. Going beyond $h = 5$ is increasingly tedious as the number of terms in equations like Eq. (9) increases rapidly. The number of equations to be satisfied by the coefficients of the various polynomials, however, increases even faster. The likelihood of finding these relatively few coefficients when many more equations than variables must be satisfied seems remote, but cannot rigorously be disproven. The discussion suggests, however, that the connection between helical curve motion and soliton equations found by Lamb² is accidental, and cannot be extended to higher order than $h = 2$ for the nonlinear Schrödinger and $h = 3$ for the modified Korteweg-de-Vries equations.

In conclusion, scaling invariance of vortex motion equations only allows the scaling of Eq. (7c) for the dependent variable in the associated nonlinear evolution equations. Scaling invariance consistent with physically acceptable vortex motion allows the nonlinear Schrödinger equation only. It is furthermore suggested that helical motion can be connected only to those nonlinear evolution equations already found by Lamb.²

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Asymptotic eigenfrequency distribution for even-parity perturbations of hot perfect-fluid relativistic neutron stars^{a)}

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Making two assumptions regarding the analytical continuation of the external solution to the region $\text{Im}\omega < 0$, we give the asymptotic distribution for $\omega \rightarrow \infty$ of the eigenfrequencies of a hot perfect fluid relativistic neutron star. It results that the real parts of the complex eigenfrequencies grow as the integers, while their imaginary parts grow as $\ln|\omega_r|$ with coefficients depending inversely on the "optical path" of the uncoupled gravitational waves through the star.

1. INTRODUCTION

In a previous paper,¹ hereafter referred to as I, we set up two systems of integral equations for even parity perturbations of perfect fluid neutron stars; their solutions describe coupled sound and gravitational waves of given frequency ω , in the framework of a single multipole of order $l \geq 2$.

The two solutions of such equations are linearly combined in order to obtain the physical solution (up to a multiplicative constant) by the requirement that the Lagrangian variation of the pressure vanishes on the star surface.

In that paper we gave an argument suggesting that the coupling between the two kinds of waves becomes weaker and weaker for $\omega \rightarrow \infty$, whereas the successive iterations furnish successive approximations to the solutions in such a limit.

In the present paper, we will prove this statement and explicitly give the physically significant internal solution for $\omega \rightarrow \infty$.

The linear combination expressing the physical solution u for the gravitational amplitude contains terms whose absolute value is proportional to $\exp|\text{Im}\omega|W_s$.² However, as a result of cancellations, the physical solution can be rewritten as a linear combination of terms whose order of magnitude is less than or equal to $\exp|\text{Im}\omega|W_g \leq \exp|\text{Im}\omega|W_s$.² A part of this paper is devoted to the proof that such cancellations occur at any order in the successive iterations. To this aim we define here new "zero order iterations" which are given by systems of integral equations including gravitational and matter field "self-interactions." In this way new integral equations, which take into account only the coupling between sound and gravitational waves, are constructed and from them the physically significant

solution is derived. The advantage of this new method lies in the fact that it makes it easier to prove the aforementioned cancellations. After this proof is worked out the computation of the dominant terms in u which do not cancel turns out to be straightforward.

The significant internal solution allows us to determine the asymptotic distribution of the eigenfrequencies in the upper ω plane, provided two reasonable assumptions (whose validity will be the object of a subsequent paper) is made on the analytical continuation of the external solution in the lower ω plane.

In fact, the knowledge of such continuation is necessary since the eigenfrequencies coincide with the zeroes of $W(-\omega)$, where W is the Wronskian function constructed with the external and gravitational solution at the star surface.³ In the framework of the cited assumptions it is found that, in the region $\text{Im}\omega > 0$, the distribution turns out to be very similar to that of the poles of the S matrix for the scattering of a particle in a potential field in quantum mechanics, when the potential is truncated or decreases at least more than any exponential.^{4,5}

The plan of the paper is the following:

In Sec. 2 we give the modified integral equations for the internal solutions, whose zero order iterations take into account the sound and gravitational "self-coupling."

In Sec. 3 majorizations for such zero order iterations are given.

In Sec. 4 the amplitudes which are needed in order to construct the physical internal solution are suitably majorized.

In Sec. 5 a representation of the internal physical solution, suitable for the subsequent majorizations, is given.

In Sec. 6 it is showed that the physical internal solution, for $\omega \rightarrow \infty$, is a combination of terms whose order of magnitude is less than or equal to $\exp|\text{Im}\omega|W_g$.

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In Sec. 7 the Wronskian function is constructed and its leading terms for $\omega \rightarrow \infty$ are calculated; the asymptotic distribution of the eigenfrequencies is finally derived.

In the Appendix we set up a method of successive approximations for integrals appearing in Sec. 7.

2. MODIFIED INTEGRAL EQUATIONS FOR THE INTERNAL SOLUTIONS

The symbols which are not defined in the present context are defined in paper I.

Let us consider the following equation in $U^{(0)}$,

$$[O_1 - V_{11}]U^{(0)} = 0, \quad (2.1)$$

where the linear differential operator $O_1 - V_{11}$ is the one acting on the variable u in (I. 2. 10). Then let us introduce the integral equations [whose solutions obey (2. 1)]

$$U_g^{(0)} = u_g^{(0)} + \int_0^r g_1(r, r')(V_{11}U_g^{(0)})_{r'} dr', \quad (2.2)$$

$$U_\sigma^{(0)} = u_\sigma^{(0)} + \int_{r_0}^r g_1(r, r')(V_{11}U_\sigma^{(0)})_{r'} dr', \quad (2.3)$$

$$u_\sigma^{(0)} = \phi_g \bar{h}_i^{(\sigma)}(x_g), \quad \sigma = \text{sign}(\text{Im}\omega), \quad (2.4)$$

where ϕ_g is given by (I. 3. 20) and $x_g = \omega W_g$, W_g being given by (I. 3. 6); $\bar{h}_i^{(\sigma)}(x_g)$, defined by (I. 3. 22), satisfies the inequality⁶

$$|\bar{h}_i^{(\sigma)}(x_g)| < C \exp(-|\text{Im}\omega| W_g) [L(|x_g|)]^{-l}, \quad (2.5)$$

where $L(x) = x/(1+x)$.

$U_g^{(0)}$, $U_\sigma^{(0)}$ are respectively regular and irregular for $r=0$.

Similarly consider the following equation in $H^{(0)}$,

$$[O_2 - V_{22}]H^{(0)} = 0, \quad (2.6)$$

where the linear differential operator $O_2 - V_{22}$ is the one acting on the variable η in (I. 2. 23).

Let us introduce the integral equations [whose solutions obey (2. 6)]

$$H_s^{(0)} = \eta_s^{(0)} + \int_0^r g_2(r, r')(V_{22}H_s^{(0)})_{r'} dr', \quad (2.7)$$

$$H_\sigma = \eta_\sigma^{(0)} + \int_{r_0}^r g_2(r, r')(V_{22}H_\sigma^{(0)})_{r'} dr', \quad (2.8)$$

$$\eta_\sigma^{(0)} = \phi_s [\vartheta(r - \bar{r}) \bar{h}_i^{(\sigma)}(X) \exp[-|\text{Im}\omega| W_0] + \vartheta(\bar{r} - r) (c_+ \bar{h}_i^{(\sigma)}(x_s) + c_- \bar{h}_i^{(-\sigma)}(x_s))], \quad (2.9)$$

where ϕ_s, X, W_s, W_0 are given respectively by (I. 3. 21), (I. A13), (I. 3. 8), and $x_s = \omega W_s$; c_+, c_- are determined by imposing the continuity of $\eta_\sigma^{(0)}$ and of its derivative with respect to r at the junction point \bar{r} . One verifies that

$$|\eta_\sigma^{(0)}/\phi_s| < C \exp(-|\text{Im}\omega| W_s) \times \{\theta(\bar{r} - r) [L(|x_s|)]^{-l} + \theta(r - \bar{r}) [L(|X|)]^{-l}\}. \quad (2.10)$$

$H_s^{(0)}$ and $H_\sigma^{(0)}$ are respectively regular and irregular for $r=0$.

In comparison with paper I, $U_g^{(0)}$ and $H_s^{(0)}$ furnish new zero-order iterations for solutions of the "gravitational" and "matter field" type instead of $u_g^{(0)}$, $\eta_s^{(0)}$.

In principle they account exactly for the self-interaction terms $V_{11}u$ and $V_{22}\eta$ appearing in (I. 3. 3) and (I. 3. 4).

To be more definite, we can construct new regular solutions of the original Eqs. (I. 2. 10) and (I. 2. 23) determined by the following systems of integral equations [to be compared with (I. 3. 26) and (I. 3. 27)],

$$U_g = U_g^{(0)} + \int_0^r G_1(r, r')(V_{12}H_g)_{r'} dr', \quad (2.11)$$

$$H_g = \int_0^r G_2(r, r')(V_{21}U_g)_{r'} dr',$$

$$U_s = \int_0^r G_1(r, r')(V_{12}H_s)_{r'} dr', \quad (2.12)$$

$$H_s = H_s^{(0)} + \int_0^r G_2(r, r')(V_{21}U_s)_{r'} dr',$$

$$G_1(r, r') = -\frac{U_g^{(0)}(r)U_\sigma^{(0)}(r') - U_\sigma^{(0)}(r)U_g^{(0)}(r')}{[W(U_g^{(0)}; U_\sigma^{(0)})]_{r'}}, \quad (2.13)$$

$$G_2(r, r') = -\frac{H_s^{(0)}(r)H_\sigma^{(0)}(r') - H_\sigma^{(0)}(r)H_s^{(0)}(r')}{[W(H_s^{(0)}; H_\sigma^{(0)})]_{r'}}, \quad (2.14)$$

where $W(\psi_1, \psi_2)$ is the Wronskian constructed with ψ_1 and ψ_2 .

3. MAJORIZATION OF $U_g^{(0)}$, $U_\sigma^{(0)}$, $H_s^{(0)}$, $H_\sigma^{(0)}$

In the following, frequent use will be made of inequalities relative to the functions ϕ_g, ϕ_s implied in the definitions of $u_g^{(0)}$, $u_\sigma^{(0)}$, $\eta_s^{(0)}$, $\eta_\sigma^{(0)}$. These hold for ω large enough and are easily verified by inspection,

$$C_1 < r\phi_g < C_2, \quad (3.1)$$

$$C_1 < r(\rho + p)^{-1/2} v_s^{-1/2} \phi_s < C_2. \quad (3.2)$$

Successive iterations can be given for the Eqs. (2. 2), (2. 3)

$$U_g^{(0, n+1)} = \int_0^r g_1(r, r')(V_{11}U_g^{(0, n)})_{r'} dr', \quad (3.3)$$

$$U_\sigma^{(0, n+1)} = \int_{r_0}^r g_1(r, r')(V_{11}U_\sigma^{(0, n)})_{r'} dr', \quad (3.4)$$

$$U_g^{(0, 0)} = u_g^{(0)}, \quad U_\sigma^{(0, 0)} = u_\sigma^{(0)}. \quad (3.5)$$

Let us set

$$U_g^{(0)} = \bar{U}_g^{(0)} r^{-1} [L(|x_g|)]^{l+1} \exp[|\text{Im}\omega| W_g], \quad (3.6a)$$

$$\bar{g}_1(r, r') = g_1(r, r')(r/r') [L(|x_g|)]^{-(l+1)} \times \exp[|\text{Im}\omega| (W_g' - W_g)], \quad (3.6b)$$

$$\bar{V}_{11} = V_{11} \exp[(\nu - \lambda)/2] v_s [L(|x_g|)]^{l+1}. \quad (3.6c)$$

From (3. 3), (3. 5), and (3. 6) one obtains

$$\bar{U}_g^{(0, n)} = \int_0^W \bar{g}_1(r, r_1) \bar{V}_{11}(r_1) dW_{s1} \int_0^W \bar{g}_1(r_1, r_2) \bar{V}_{11}(r_2) dW_{s2} \dots \int_0^W \bar{g}_1(r_{n-1}, r_n) \bar{V}_{11}(r_n) \bar{U}_g^{(0, 0)} dW_{sn}. \quad (3.7)$$

Furthermore by inspection one can see that $\bar{U}_g^{(0, 0)} = \bar{u}_g^{(0)}$, $\bar{g}_1 \bar{V}_{11} = \bar{g}_1' \bar{V}_{11}'$, where $\bar{u}_g^{(0)}$, \bar{V}_{11}' , \bar{g}_1' are defined by (I. 4. 4), (I. 4. 7), (I. 4. 9). Then from (I. 4. 13), (I. 4. 14) for $r' \leq r$ we obtain

$$|\bar{g}_1(r, r') \bar{V}_{11}'(r')| < \frac{C}{|\omega|}, \quad |\bar{U}_g^{(0, 0)}| < C. \quad (3.8)$$

From the above inequalities and (3.7) we get

$$|\bar{U}_\varepsilon^{(0,n)}| < \frac{C^{n+1}W_s^m}{|\omega|^{n+1}} \quad (3.9)$$

and then from (3.6a), by summation of all iterations,

$$|U_\varepsilon^{(0)}| < Cr^{-1}[L(|x_\varepsilon|)]^{l+1} \exp[|\operatorname{Im}\omega|W_\varepsilon]. \quad (3.10)$$

In a similar way, introducing

$$U_\sigma^{(0)} = \hat{U}_\sigma^{(0)} r^{-1} [L(|x_\sigma|)]^{-l} \exp(-|\operatorname{Im}\omega|W_\sigma), \quad (3.11a)$$

$$\hat{g}_1(r, r') = g_1(r, r') [L(|x_\sigma|)]^l \exp[|\operatorname{Im}\omega|(W_\sigma - W'_\sigma)], \quad (3.11b)$$

$$\hat{V}_{11} = V_{11} \exp[(\nu - \lambda)/2] v_s [L(|x_\sigma|)]^{-l}, \quad (3.11c)$$

one can see by inspection that $\hat{g}_1 \hat{V}_{11} = \tilde{g}_1 \tilde{V}_{11} \exp[2|\operatorname{Im}\omega| \times (W_\sigma - W'_\sigma)]$,

so that, owing to (I.4.13), one obtains

$$|\hat{g}_1(r, r') \hat{V}_{11}(r')| < \frac{C}{|\omega|}, \quad r \leq r', \quad (3.12)$$

and taking into account (2.5), (3.1), and (3.11a) one obtains

$$|\hat{U}_\sigma^{(0,0)}| < C. \quad (3.13)$$

Then, with the help of the above inequality, together with (3.4) and (3.12), with a procedure quite similar to that outlined for $U_\varepsilon^{(0)}$, we get

$$|U_\sigma^{(0)}| < Cr^{-1}[L(|x_\sigma|)]^{-l} \exp(-|\operatorname{Im}\omega|W_\sigma). \quad (3.14)$$

In an analogous way the successive iterations of (2.7) and (2.8) read

$$H_s^{(0,n+1)} = \int_0^r g_2(r, r') (V_{22} H_s^{(0,n)})_{r'} dr', \quad (3.15)$$

$$H_\sigma^{(0,n+1)} = \int_0^r g_2(r, r') (V_{22} H_\sigma^{(0,n)})_{r'} dr', \quad (3.16)$$

$$H_s^{(0,0)} = \eta_s^{(0)}, \quad H_\sigma^{(0,0)} = \eta_\sigma^{(0)}. \quad (3.17)$$

Then let us introduce

$$H_s^{(0)} = \bar{H}_s^{(0)} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \quad (3.18a)$$

$$\begin{aligned} \bar{g}_2(r, r') = g_2(r, r') \frac{r}{r'} \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|(W'_s - W_s)], \end{aligned} \quad (3.18b)$$

$$\bar{V}_{22} = V_{22} e^{(\nu - \lambda)/2} v_s \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \quad (3.18c)$$

and

$$H_\sigma^{(0)} = \hat{H}_\sigma^{(0)} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp(-|\operatorname{Im}\omega|W_\sigma), \quad (3.19a)$$

$$\begin{aligned} \hat{g}_2(r, r') = g_2(r, r') \frac{r}{r'} \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \{ \theta(\bar{r} - r) [L(|x_s|)]^l \\ + \theta(r - \bar{r}) [L(|X|)]^l \} \exp[|\operatorname{Im}\omega|(W_s - W'_\sigma)], \end{aligned} \quad (3.19b)$$

$$\begin{aligned} \hat{V}_{22} = V_{22} \exp[(\nu - \lambda)/2] v_s \{ [L(|x_s|)]^{-l} \theta(\bar{r} - r) \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \}. \end{aligned} \quad (3.19c)$$

Now one can verify that $\bar{H}_s^{(0,0)} = \tilde{\eta}_s^{(0)}$, $\bar{g}_2 \bar{V}_{22} = \tilde{g}_2 \tilde{V}_{22}$, and

$$\tilde{g}_2 \hat{V}_{22} = \tilde{g}_2 \tilde{V}_{22} \exp[2|\operatorname{Im}\omega|(W_s - W'_\sigma)],$$

where $\tilde{\eta}_s^{(0)}$, \tilde{V}_{22} , and \tilde{g}_2 are defined by (I.4.5), (I.4.8), and (I.4.10). Then from (I.4.13) and (I.4.14) it follows that:

$$|\bar{g}_2(r, r') \bar{V}_{22}(r')| < \frac{C}{|\omega|}, \quad r' \leq r, \quad (3.20)$$

$$|\hat{g}_2(r, r') \hat{V}_{22}(r')| < \frac{C}{|\omega|}, \quad r \leq r', \quad (3.21)$$

$$|\bar{H}_s^{(0,0)}| < C. \quad (3.22)$$

In addition, an inequality similar to (3.13) is easily derived,

$$|\hat{H}_\sigma^{(0,0)}| < C. \quad (3.23)$$

Finally, with a procedure similar to that outlined in order to obtain (3.10) and (3.14), we get

$$\begin{aligned} |H_s^{(0)}| < Cr^{-1} (W_0 - W_s)^l \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \end{aligned} \quad (3.24)$$

$$\begin{aligned} |H_\sigma^{(0)}| < Cr^{-1} (W_0 - W_s)^l \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp(-|\operatorname{Im}\omega|W_\sigma). \end{aligned} \quad (3.25)$$

4. MAJORIZATIONS OF H_g, H_s

A program parallel to that of Sec. 4 of paper I can now be developed for the coupled integral equations (2.11) and (2.12); however, in the present context, we are interested only in the amplitudes H . Let us set

$$\begin{aligned} H = \bar{H} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \end{aligned} \quad (4.1)$$

$$U = \tilde{U} r^{-1} [L(|x_s|)]^{l+1} \exp[|\operatorname{Im}\omega|W_s], \quad (4.2)$$

$$\tilde{G}_1(r, r') = G_1(r, r') \frac{r}{r'} [L(|x_s|)]^{-l+1} \exp[|\operatorname{Im}\omega|(W'_s - W_s)], \quad (4.3)$$

$$\begin{aligned} \tilde{G}_2(r, r') = G_2(r, r') \frac{r}{r'} \exp[|\operatorname{Im}\omega|(W'_s - W_s)] \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \\ \times \{ [L(|x_s|)]^{-l+1} \theta(\bar{r} - r) + \theta(r - \bar{r}) [L(|X|)]^{-l} \}. \end{aligned} \quad (4.4)$$

We want to prove now that

$$|\tilde{G}_1(r, r') \tilde{V}_{12}(r')| < \frac{C}{|\omega|^3}, \quad (4.5)$$

$$|\tilde{G}_2(r, r') \tilde{V}_{21}(r')| < \frac{C}{|\omega|^3}, \quad (4.6)$$

where $\tilde{V}_{12}, \tilde{V}_{21}$ are defined by (I.4.7), (I.4.8).

In order to do this it is necessary to give suitable majorizations of $G_1(r, r')$ and $G_2(r, r')$, given by (2.13) and (2.14), and therefore, among other things, to assign minorizations of the Wronskians appearing in them.

From (2.2) and (2.3) one gets

$$\begin{aligned}
 & W(U_g^{(0)}; U_o^{(0)}) \\
 &= W(u_g^{(0)}; u_o^{(0)}) \left[1 + \omega^{-1} \int_0^r \frac{u_o^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \right. \\
 &\quad - \omega^{-1} \int_0^r \frac{u_g^{(0)} V_{11} U_o^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \\
 &\quad - \omega^{-2} \int_0^r \frac{u_o^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \int_{r_0}^r \frac{u_g^{(0)} V_{11} U_o^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \\
 &\quad \left. + \omega^{-2} \int_0^r \frac{u_g^{(0)} V_{11} U_o^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \int_{r_0}^r \frac{u_o^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \right]. \quad (4.7)
 \end{aligned}$$

Taking into account the inequality $|V_{11}| < C$, quoted in the appendix of paper I, and making use of (3.1), (3.6a), (3.8), (3.11a), (3.13), and (3.14) one obtains

$$|W(U_g^{(0)}; U_o^{(0)})| > Cr^{-2} |\omega|. \quad (4.8)$$

In a similar way one can minorize the Wronskian appearing in $G_2(r, r')$ making use of (3.2), (3.18a), (3.22), (3.19a), (3.23), (3.24), and (3.25) together with (I.3.15)

$$\begin{aligned}
 & W(H_s^{(0)}; H_o^{(0)}) W(\eta_s^{(0)}; \eta_o^{(0)}) \left(1 + \frac{Q}{\omega} \right) \\
 &= -\omega \phi_s^2 \frac{\exp(\lambda - \nu)/2}{v_s}, \quad |Q| < C, \quad (4.9)
 \end{aligned}$$

$$|W(H_s^{(0)}; H_o^{(0)})| > Cr^{-2}(\rho + p) |\omega|.$$

Taking into account that V_{21} and V_{12} , given by (I.3.11), are respectively proportional to $(\rho + p)\omega^{-4}$ and ω^{-2} , from (3.10), (3.14), (3.24), (3.25), (4.8), and (4.9), we straightforwardly get the inequalities (4.5) and (4.6).

Comparing (4.1), (4.2) respectively with (3.18a), (3.6a) we get by means of (3.24), (3.10),

$$|\tilde{H}_s^{(0)}| = |\bar{H}_s^{(0)}| < C, \quad (4.10)$$

$$\begin{aligned}
 |\tilde{U}_g^{(0)}| &= |\bar{U}_g^{(0)}| [L(|x_g|)/L(|x_s|)]^{l+1} \exp[|\operatorname{Im}\omega| (W_g - W_s)] \\
 &< C. \quad (4.11)
 \end{aligned}$$

Finally from (2.11), (2.12) together with (4.1), (4.2), one gets

$$\begin{aligned}
 \tilde{H}_g^{(n)} &= \frac{1 - (-1)^n}{2} \int_0^W \tilde{G}_2(r, r_1) \tilde{V}_{21}(r_1) dW_{s_1} \\
 &\quad \times \int_0^{W_{s_1}} \tilde{G}_1(r_1, r_2) \tilde{V}_{12}(r_2) dW_{s_2} \dots \\
 &\quad \int_0^{W_{s_{n-1}}} \tilde{G}_2(r_{n-1}, r_n) \tilde{V}_{21}(r_n) \tilde{U}_g^{(0)}(r_n) dW_{s_n}, \quad (4.12)
 \end{aligned}$$

$$\begin{aligned}
 \tilde{H}_s^{(n)} &= \frac{1 + (-1)^n}{2} \int_0^W \tilde{G}_2(r, r_1) \tilde{V}_{21}(r_1) dW_{s_1} \\
 &\quad \times \int_0^{W_{s_1}} \tilde{G}_1(r_1, r_2) \tilde{V}_{12}(r_2) dW_{s_2} \dots \\
 &\quad \int_0^{W_{s_{n-1}}} \tilde{G}_1(r_{n-1}, r_n) \tilde{V}_{12} \tilde{H}_s^{(0)}(r_n) dW_{s_n}. \quad (4.13)
 \end{aligned}$$

From these and from (4.5), (4.6), (4.10), and (4.11) it follows that

$$|\tilde{H}_g^{(n)}| < \frac{C^{n+1} W_s^m}{n! |\omega|^{4n+1}}, \quad (4.14)$$

$$|\tilde{H}_s^{(n)}| < \frac{C^{n+1} W_s^m}{n! |\omega|^{4n}}, \quad (4.15)$$

and then, in analogy with (I.4.16),

$$\begin{aligned}
 \left| \sum_{n=0}^{\infty} \left[\frac{H_g^{(n)}}{H_s^{(n)}} \right] \right| &< r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\
 &\quad + [L(|X|)]^{-l} \theta(r - \bar{r}) \} \exp[|\operatorname{Im}\omega| W_s] \\
 &\quad \times \frac{C^{m+1} W_s^m}{m! |\omega|^m} \exp\left(\frac{CW_0}{|\omega|}\right). \quad (4.16)
 \end{aligned}$$

5. REPRESENTATION OF THE PHYSICAL SOLUTION

In analogy with (I.3.30), (I.3.31), and (I.3.32), the physical solution can be alternatively written as⁷

$$u = U_g + \mu_1 U_s, \quad (5.1)$$

$$\eta = H_g + \mu_1 H_s, \quad (5.2)$$

$$\mu_1 = -(H_g/H_s)_{r_0}; \quad (5.3)$$

it follows that

$$\begin{aligned}
 u &= (H_s(r_0) U_g - U_s H_g(r_0)) \frac{1}{H_s(r_0)} \\
 &= \frac{1}{H_s(r_0)} \sum_{n=0}^{\infty} \sum_{j=0}^n [H_s^{(j)}(r_0) U_g^{(n-j)} - U_s^{(j)} H_g^{(n-j)}(r_0)]. \quad (5.4)
 \end{aligned}$$

Now (4.12) and (4.13) imply the relations $H_g^{(2n)} = H_s^{(2n+1)} = 0$, which also lead to $U_g^{(2n+1)} = U_s^{(2n)} = 0$ by iteration of (2.11) and (2.12). Then we get

$$\begin{aligned}
 u &= \frac{1}{H_s(r_0)} \sum_{n=0}^{\infty} \left[\theta(2n-1) \left(\sum_{j=0}^{2n-1} H_s^{(j)}(r_0) U_g^{(2n-j)} \right) \right. \\
 &\quad \left. - \sum_{j=1}^{2n} U_s^{(j)} H_g^{(2n-j)}(r_0) \right] + H_s^{(2n)}(r_0) U_g^{(0)}. \quad (5.5)
 \end{aligned}$$

Introducing in (5.5) the iterations of (2.11) and (2.12) for U_g and U_s we further obtain

$$u = U_g^{(0)} + \sum_{n=1}^{\infty} S^{(n)}, \quad (5.6)$$

$$S^{(n)} = \frac{1}{H_s(r_0)} \int_0^r G_1(r, r') V_{12}(r') \Lambda^{(2n-1)}(r_0, r') dr', \quad (5.7)$$

$$\begin{aligned}
 \Lambda^{(n)}(r_0, r') &= \sum_{j=0}^{n-1} [H_s^{(2j)}(r_0) H_g^{(2n-2j-1)}(r') \\
 &\quad - H_s^{(2j)}(r') H_g^{(2n-2j-1)}(r_0)]. \quad (5.8)
 \end{aligned}$$

Now, as stated in Sec. 1, we want to show that u is proportional to $\exp|\operatorname{Im}\omega| W_g$ despite the fact that most of the terms appearing in it behave like $\exp|\operatorname{Im}\omega| W_s$. In order to do this a suitable representation of the expressions in the square brackets is necessary.

Let us define

$$k = - \int_0^r \frac{H_o^{(0)} V_{21} U_g^{(0)}}{W(H_s^{(0)}; H_o^{(0)})} dr', \quad (5.9)$$

$$I_1(r, r') = \frac{H_s^{(0)}(r) H_o^{(0)}(r') V_{21}(r')}{[W(H_s^{(0)}; H_o^{(0)})]_{r'}}, \quad (5.10)$$

$$I_2(r, r') = \frac{H_o^{(0)}(r) H_s^{(0)}(r') V_{21}(r')}{[W(H_s^{(0)}; H_o^{(0)})]_{r'}}, \quad (5.11)$$

$$f_1(r) = \int_r^{r_0} I_1(r, r') U_g^{(0)}(r') dr' + \int_0^r I_2(r, r') U_g^{(0)}(r') dr', \quad (5.12)$$

$$f_2(r) = \int_0^r G_1(r, r') (V_{12} f_1)_{r'} dr', \quad (5.13)$$

$$\dots \dots \dots f_{2n+1}(r) = \int_r^{r_0} I_1(r, r') f_{2n}(r') dr' + \int_0^r I_2(r, r') f_{2n}(r') dr', \quad (5.14)$$

$$f_{2n+2}(r) = \int_0^r G_1(r, r') (V_{12} f_{2n+1})_{r'} dr'. \quad (5.15)$$

From (5.9)–(5.12) we get

$$\int_0^r G_2(r, r') (V_{21} U_g^{(0)})_{r'} dr' = k H_s^{(0)} + f_1. \quad (5.16)$$

Then for the terms $H_s^{(2j)}(r_0) H_g^{(2n-2j-1)}(r)$ appearing in (5.8), taking into account (5.16), we can write

$$H_s^{(0)}(r_0) H_g^{(2n-1)} = H_s^{(0)}(r_0) k H_s^{(2n-2)} + H_s^{(0)}(r_0) \times \int_0^r G_2(r, r_1) V_{21}(r_1) dr_1 \int_0^{r_1} G_1(r_1, r_2) V_{12}(r_2) dr_2 \dots \int_0^{r_{2n-3}} G_1(r_{2n-3}, r_{2n-2}) (V_{12} f_1)_{r_{2n-2}} dr_{2n-2}, \quad (5.17)$$

$$H_s^{(2)}(r_0) H_g^{(2n-3)} = H_s^{(2)}(r_0) k H_s^{(2n-4)} + H_s^{(2)}(r_0) \int_0^r G_2(r, r_1) V_{21}(r_1) dr \times \int_0^{r_1} G_1(r_1, r_2) V_{12}(r_2) dr_2 \dots \int_0^{r_{2n-5}} G_1(r_{2n-5}, r_{2n-4}) (V_{12} f_1)_{r_{2n-4}} dr_{2n-4}, \quad (5.18)$$

$$\dots \dots \dots H_s^{(2n-4)}(r_0) H_g^{(3)} = k H_s^{(2n-4)}(r_0) H_s^{(2)} + H_s^{(2n-4)}(r_0) \int_0^r G_1(r, r_1) (V_{12} f_1)_{r_1} dr_1, \quad (5.19)$$

$$H_s^{(2n-2)}(r_0) H_g^{(1)} = k H_s^{(2n-2)}(r_0) H_s^{(0)} + H_s^{(2n-2)}(r_0) f_1. \quad (5.20)$$

Quite similar relations can be obtained for the counterterms in (5.8) from the above ones by means of the exchange $r \rightarrow r_0$ in the arguments of $H_s^{(i)}$ and f_1 . In the sum appearing in (5.8), terms and counterterms proportional to k cancel one another; more precisely, the first term cancels the last counterterm, the second term cancels the last but one counterterm, and so on. The sum of the remaining terms can be written as

$$H_s^{(2n-2)}(r_0) f_1 - H_s^{(2n-2)} f_1(r_0) + \left[\sum_{j=0}^{n-3} (H_s^{(2j)}(r_0) H_g^{(2n-2j-3)} - H_s^{(2j)} H_g^{(2n-2j-3)}(r_0)) \right] U_g^{(0)} - f_2, \quad (5.21)$$

where it is understood that the formal replacement $U_g^{(0)} \rightarrow f_2$ has to be made in the integrals expressing any $H_g^{(v)}$. The sum appearing in the above expression is similar to that relative to (5.8) with the substitution $n \rightarrow n-1$. Taking into account (5.14) and (5.15) at any

step we finally obtain

$$\Lambda^{(n)}(r_0, r') = \sum_{j=0}^{n-1} (H_s^{(n-j-1)}(r_0) f_{2j+1}(r') - H_s^{(n-j-1)}(r') f_{2j+1}(r_0)), \quad (5.22)$$

which, by means of (5.6) and (5.7), allows us to get the final expression for u .

6. MAJORIZATION FOR $S^{(n)}$

From (5.10) and (5.11) together with (3.10), (3.24), (3.25), and (4.8) one gets

$$|f_1(r)| < \frac{C_0 C_1 r^{-1}}{|\omega|^5} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g], \quad (6.1)$$

where C_0 denotes a determination of the constant C appearing in (3.10).

Now from (3.10), (3.14), and (4.8) we obtain a majorization for $G_1(r, r')$ which is the same as (I. A6); making use of such majorization together with $|V_{12}| < C|\omega|^{-2}$ in (5.13), we can write

$$|f_2(r)| < \frac{C_0 C_1 C_2 r^{-1}}{|\omega|^8} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g]. \quad (6.2)$$

The majorization procedure can now be extended straightforwardly to (5.14),

$$\left| \frac{f_{2n+1}}{r^{-1} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g]} \right| < \frac{C_0 C_1 (C_1 C_2)^n}{|\omega|^{8n+5}} < \frac{C^{2n+2}}{|\omega|^{8n+5}}, \quad (6.3)$$

where C is the largest constant among $C_0, C_1,$ and C_2 .

Again taking into account the above cited majorizations for $G_1(r, r'), V_{12}$ and making use of (6.3), (4.15), (4.1), (3.10), and (5.7), one gets

$$|S^{(n)}| < \frac{C^{n+2}}{|\omega|^{8n}} [L(|x_g|)]^{l+1} n C \frac{\exp[|\operatorname{Im} \omega| (W_g + W_0)]}{|H_s(r_0)|}. \quad (6.4)$$

From the above inequality and from (5.6) it follows that

$$\left| \sum_{n=m}^{\infty} S^{(n)} \right| < \frac{C^2 \xi^m}{H_s(r_0)} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| (W_g + W_0)] \times C \left(\frac{\xi}{(1-\xi)^2} + \frac{m}{1-\xi} \right), \quad (6.5)$$

$$\xi = C/|\omega|^8. \quad (6.6)$$

From the results of Secs. 3 and 4 it follows that⁸

$$H_s(r_0) \approx H_s^{(0)}(r_0) \approx \eta_s^{(0)}(r_0), \quad (6.7)$$

and then from the explicit evaluation of $\eta_s^{(0)}(r_0)$ by means of (I. 3.18),

$$|H_s(r_0)| \approx |\eta_s^{(0)}(r_0)| \approx \frac{C \exp[|\operatorname{Im} \omega| W_0]}{|\omega|^{\bar{r}}}. \quad (6.8)$$

So from (6.4), (6.7), and (6.8) one sees that u near the star surface is proportional to $\exp[|\operatorname{Im} \omega| W_g(r_0)]$ times powers of ω^{-1} .

7. ZEROES OF THE WRONSKIAN

Let us now consider the Wronskian $W(u, u_-)$, whose zeroes give the eigenfrequencies of the star.

From (5.6)–(5.8), recalling the transformation property of the Wronskian for two independent solutions of a second order linear differential equation, we obtain

$$W(u, u_-) = W(U_g^{(0)}, u_-) - \frac{1}{H_s(r_0)} \times \sum_{n=1}^{\infty} \int_0^r \frac{(u_- V_{12})_{r'} \Lambda^{(n)}(r_0, r')}{\exp(\int_{r'}^r B_1(r'') dr'')} dr', \quad (7.1)$$

where B_1 is the coefficient of u' in (I.2.10). The external amplitude u_- is defined by the integral equation (I.5.3) only for $\text{Im}\omega \geq 0$, so that the analytical continuation of u_- to the region $\text{Im}\omega < 0$ is necessary in order to evaluate $W(u, u_-)$ everywhere.

Making use of (I.5.3) and recalling that $U_g^{(0)}$ and $u_g^{(0)}$ are respectively solutions of (2.1) and (I.3.16), we get

$$W(U_g^{(0)}, u_-) = W(u_g^{(0)}, u_-^{(0)}) \left[1 + \frac{\Gamma(\omega)}{\omega} \right], \quad (7.2)$$

$$\Gamma(\omega) = -\omega \int_0^{\infty} \frac{u_g^{(0)} V_{11} u_-}{W(u_g^{(0)}; u_-^{(0)})} dr. \quad (7.3)$$

As shown in paper I, in the region $\text{Im}\omega \geq 0$ we have

$$u_- = u_-^{(0)} + o(u_-^{(0)}), \quad \omega \rightarrow \infty. \quad (7.4)$$

Recalling the definition of $u_g^{(0)}$, u_- and using a standard relation between Bessel functions of order l we get

$$W(u_g^{(0)}; u_-^{(0)}) = -\omega \phi_g^2 \exp[(\lambda - \nu)/2]. \quad (7.5)$$

Moreover, introducing for them majorizations similar to (3.10) and (3.14) we obtain for $\text{Im}\omega \geq 0$

$$|\Gamma(\omega)| < C, \quad \omega \rightarrow \infty. \quad (7.6)$$

Let us now assume that the above inequality, together with (7.3), also holds for $\text{Im}\omega < 0$.

The proof of the validity of such assumptions rests on the possibility of analytical continuation of u_- and will be the object of another paper. The extension of (7.4) to the half-plane $\text{Im}\omega < 0$ amounts to stating that the asymptotic expression of the analytical continuation is given by the continuation of the asymptotic expression.

We report the results of the asymptotic calculation of the term $n=1$; this is obtained with the help of integration techniques developed in the Appendix, together with the following equality (which derives from standard relations among Bessel functions),

$$\frac{\eta_s^{(0)} \eta_{\sigma, l+1}^{(0)} - \eta_{s, l+1}^{(0)} \eta_{\sigma}^{(0)}}{W(\eta_s^{(0)}; \eta_{\sigma}^{(0)})} = -\nu_s \frac{\exp[(\nu - \lambda)/2]}{\omega}, \quad (7.7)$$

where

$$\eta_{\sigma, l+1}^{(0)} = \phi_{s,l} \left\{ \theta(r - \bar{r}) \exp(-|\text{Im}\omega| W_0) \bar{h}_{l+1}^{(0)}(X) + \theta(\bar{r} - r) [c_s \bar{h}_{l+1}^{(0)}(x_s) + c \bar{h}_{l+1}^{(0)}(x_s)] \right\}. \quad (7.8)$$

We express $\Lambda^{(1)}(r, r')$ by means of (5.22), taking $n=1$, $j=0$, together with (5.10)–(5.12).

Let us write

$$\Lambda^{(1)}(r, r') = \Lambda_0^{(1)}(r, r') + R_A^{(1)}(r, r'); \quad (7.9)$$

$\Lambda_0^{(1)}$ is the “zero order approximation” for $\Lambda^{(1)}$ in the sense specified in the Appendix, evaluated with the substitutions

$$U_g^{(0)} - U_g^{(0,0)} = u_g^{(0)}, \quad U_{\sigma}^{(0)} - U_{\sigma}^{(0,0)} = u_{\sigma}^{(0)}, \\ H_s^{(0)} - H_s^{(0,0)} = \eta_s^{(0)}, \quad H_{\sigma}^{(0)} - H_{\sigma}^{(0,0)} = \eta_{\sigma}^{(0)}, \quad (7.10)$$

In the numerators of (5.10) and (5.11).

$R_A^{(1)}(r, r')$ is comprehensive both of the higher order iterations describing self-interactions and of remainders to integrals involved in (5.12) together with (7.10) and (7.11).

Similar considerations can be also made for the successive integral $I^{(1)}$ implied in (7.1) in the case $n=1$; again its zero order approximation $I_0^{(1)}$ is obtained by means of the substitution $\Lambda^{(1)}(r, r') - \Lambda_0^{(1)}(r, r')$ together with the substitutions (7.10) in the numerator of $G_1(r, r')$, given by (2.13).

Using (3.10), (3.14), (3.24), (3.25), (4.8), (4.9), and (3.9) together with analogous relations for $U_{\sigma}^{(0,n)}$, $H_s^{(0,n)}$, $H_{\sigma}^{(0,n)}$, it is long, but without difficulties and completely in the spirit of the majorization procedures outlined in Sec. 3, to show that the following quantities are negligible for $\omega \rightarrow \infty$ in the expression between brackets in (7.1):

- (i) The integral implying $R_A^{(1)}(r, r')$;
- (ii) The remainder to $I_0^{(1)}$ in the sense of the Appendix;
- (iii) The contributions to $I^{(1)}$ arising from the neglected terms in $G_1(r, r')$, which describe self-interactions;
- (iv) The overall contribution $\sum_{n=2}^{\infty} I^{(n)}$, arising from terms of order $n > 1$;

The calculations lead to

$$I^{(1)} \approx I_0^{(1)} \approx \frac{1}{2\omega} \eta_s^{(0)} \phi_g^2 \left[\bar{j}_l(x_g) \left(\bar{h}_l^{(*)}(x_g) - \frac{l+1}{x_g} \bar{h}_{l+1}^{(*)}(x_g) \right) + \bar{j}_{l+1}(x_g) \left(\bar{h}_{l+1}^{(*)}(x_g) - \frac{l+1}{x_g} \bar{h}_l^{(*)}(x_g) \right) \right] \times \int_0^{w_g(r_0)} \frac{V_{12} V_{21} \nu_s \exp(\nu - \lambda)}{(1 - \nu_s^2) W(H_s^{(0)}, H_{\sigma}^{(0)})} dW_g. \quad (7.11)$$

So let us introduce (7.11) together with (4.9) and (6.7) in (7.1) and replace for $\bar{h}_l^{(*)}(x_g)$ and $\bar{j}_l(x_g)$ ($\nu=l$, $l+1$) their asymptotic expressions for $x_g \rightarrow \infty$.

Then, recalling that $V_{12} V_{21} \sim \omega^{-6}$ and changing sign to ω according to the final remark made in Sec. 1, in the framework of the assumptions we have done, we conclude that the asymptotic eigenfrequencies of the star are given by the equation

$$1 + \frac{\alpha}{i\omega} \exp[-2i\omega W_g(r_0)] = 0, \quad (7.12)$$

where the real ω -independent constant α is given by

$$\alpha = (-1)^{l+1} \frac{l+1}{2} \left(\frac{\exp[(\nu - \lambda)/2]}{W_\varepsilon^2} \right) \times \int_0^{W_\varepsilon(r_0)} \frac{(\lim_{\omega \rightarrow \infty} V_{12} V_{21} \omega^6) \exp[3(\nu - \lambda)/2]}{\phi_s^2[(1/\nu_s) - 1]} dW_\varepsilon. \quad (7.13)$$

The zeroes of (7.12) are symmetrically distributed with respect to the imaginary axis, and for $\text{Re}\omega > 0$ are asymptotically given by

$$\text{Re}\omega_n \approx \frac{(2n + \frac{1}{2})\pi + \arg\alpha}{2W_\varepsilon(r_0)}, \quad (7.14)$$

$$\text{Im}\omega_n \approx \frac{11 \ln|\text{Re}\omega_n| \text{Re}\omega_n - \ln|\alpha|}{2W_\varepsilon(r_0)}, \quad (7.15)$$

where n is an arbitrary integer such that the rhs of (7.14) is positive. As seen from the above results, the dependence of the ω_n 's on the coupling between the sound and the gravitational waves (contained in α) is weak.

8. FINAL REMARKS

The eigenfrequencies are equally spaced with respect to the real axis of the ω plane and are distributed along a logarithmic curve.

This is also the case for the energy eigenvalues of a particle in a spherically symmetric truncated potential in wave mechanics.⁵

It is easy to see that a similar distribution also occurs in the simpler case of a system⁹ made of two uniform parallel strings of different nature coupled together with transversal uniformly distributed identical springs according to Fig. 1, where A, B , and C are fixed points and string 1 is indefinite towards the right.

The system can be compared with a neutron star radiating gravitational waves; to be definite, strings 1 and 2 can be respectively compared with the physical space (thought of as the medium which propagates the gravitational radiation) and the matter in the star (through which sound waves are propagated). We note that in our case the asymptotic distribution of the eigenfrequencies depends on the equilibrium structure essentially through $W_\varepsilon(r_0)$, which can be interpreted as the optical path of the (uncoupled) gravitational waves throughout the star. With the constant α is associated only a finite "displacement," which is the same for the various eigenfrequencies.

Another observation, which may be relevant for the completeness of eigenmodes, is that the asymptotic zeroes are simple.

APPENDIX

The aim of this appendix is to give a method of successive approximations for large values of $|\omega|$, for integrals which are involved in the iterations for U, H ;

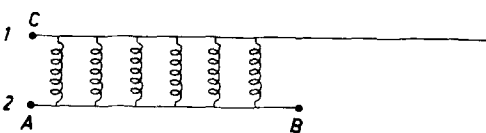


FIG. 1. Coupled springs simulating the interaction of the gravitational field with the neutron star matter.

these belong to the general type

$$I = \int_a^x [A^{(0)} \varphi_l(\omega \Phi_1) \bar{\varphi}_{l'}(\omega \Phi_2) + B^{(0)} \varphi_{l+1}(\omega \Phi_1) \bar{\varphi}_{l'}(\omega \Phi_2) + C^{(0)} \varphi_l(\omega \Phi_1) \bar{\varphi}_{l'+1}(\omega \Phi_2) + D^{(0)} \varphi_{l+1}(\omega \Phi_1) \bar{\varphi}_{l'+1}(\omega \Phi_2)]_x dx', \quad (A1)$$

where $a=0$ or ∞ respectively, for internal and external solutions, $\varphi_{l+j}, \bar{\varphi}_{l'+j_1}$ ($j, j_1=0, 1$) denote the product of spherical Bessel functions of order $l+j, l'+j_1$ times their respective arguments $\omega \Phi_1$ and $\omega \Phi_2$, Φ_1 and Φ_2 being functions of x only; $A^{(0)}, B^{(0)}, C^{(0)}$, and $D^{(0)}$ are functions of x and ω ; we assume that in the limit $\omega \rightarrow \infty$ these are "slowly varying" functions of x , compared with $\varphi_{l+j}, \bar{\varphi}_{l'+j_1}$, which exhibit an exponential behavior of the type $\exp(i\omega \Phi_k)$; it must be understood that φ_l and φ_{l+1} are constructed with Bessel functions of the same kind, namely the coefficients of the linear combination expressing φ_{l+1} in terms of j_{l+1} and n_{l+1} , are the same as those relative to the linear combination expressing φ_l in terms of j_l, n_l ; similarly, $\varphi_{l'}$ and $\varphi_{l'+1}$ are of the same kind (though this may be different from that relative to φ_l, φ_{l+1}). Let us first consider the case $\Phi_1 \neq \Phi_2$, to be distinguished from the case $\Phi_1 = \Phi_2$. For the primitive relative to the integral (A1) we shall tentatively assume a form similar to the integrand

$$P = a \varphi_l \bar{\varphi}_{l'} + b \bar{\varphi}_{l'+1} \varphi_{l'} + c \varphi_l \bar{\varphi}_{l'+1} + d \varphi_{l+1} \bar{\varphi}_{l'+1}, \quad (A2)$$

where a, b, c , and d are to be determined by a method of successive approximations. Owing to a property of Bessel functions, we have

$$\frac{d\varphi_l}{dx} = \omega \frac{d\Phi_1}{dx} \left(-\varphi_{l+1} \frac{l+1}{\omega \Phi_1} \varphi_l \right), \quad (A3)$$

$$\frac{d\varphi_{l+1}}{dx} = \omega \frac{d\Phi_1}{dx} \left(\varphi_l - \frac{l+1}{\omega \Phi_1} \varphi_{l+1} \right),$$

and similar relations for $\bar{\varphi}_{l'}, \bar{\varphi}_{l'+1}$. Then the derivative of P with respect to x can be written as a sum S of terms, originating from the first terms in the rhs's of (A3) (explicitly proportional to ω), plus other terms whose sum we denote by $-T$.

In our problem, in the interval $0 \leq r \leq \bar{r}$, we have the case $l'=l, \Phi_1 = W_\varepsilon, \Phi_2 = W_s$; in such case we choose the zero order approximation $a^{(0)}, b^{(0)}, c^{(0)}$, and $d^{(0)}$ for a, b, c , and d identifying S with the integrand of (A1); in this way one gets

$$a^{(0)} = (\omega F)^{-1} (\Phi_1' B^{(0)} - \Phi_2' C^{(0)})$$

$$b^{(0)} = -(\omega F)^{-1} (\Phi_1' A^{(0)} + \Phi_2' D^{(0)}) \quad (A4)$$

$$c^{(0)} = (\omega F)^{-1} (\Phi_1' D^{(0)} + \Phi_2' A^{(0)})$$

$$d^{(0)} = -(\omega F)^{-1} (\Phi_1' C^{(0)} - \Phi_2' B^{(0)}),$$

$$F = (\Phi_2')^2 - (\Phi_1')^2, \quad \Phi_1' = \frac{d\Phi_1}{dx}, \quad \Phi_2' = \frac{d\Phi_2}{dx}, \quad (A5)$$

$$I = [a^{(0)} \varphi_l \bar{\varphi}_{l'} + b^{(0)} \varphi_{l+1} \bar{\varphi}_{l'} + c^{(0)} \varphi_l \bar{\varphi}_{l'+1} + d^{(0)} \varphi_{l+1} \bar{\varphi}_{l'+1}]_a^x + \int_a^x T dr'. \quad (A6)$$

Now the integral in the rhs of the above equality has a structure which is similar to that of the original integral (A1); however its coefficients, compared with

$A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$, exhibit an explicit factor $1/\omega$ as seen from (A4); we can therefore apply a similar procedure to such an integral, and so on. In this way one obtains a method of successive approximations for I when $|\omega|$ is large. The m th approximation is written as:

$$I = \sum_{n=0}^m [a^{(n)} \varphi_1 \bar{\varphi}_1 + b^{(n)} \varphi_{l+1} \bar{\varphi}_1 + c^{(n)} \varphi_1 \bar{\varphi}_{l+1} + d^{(n)} \varphi_{l+1} \bar{\varphi}_{l+1}]_a^x + \int_a^x [A^{(m+1)} \varphi_1 \bar{\varphi}_1 + B^{(m+1)} \varphi_{l+1} \bar{\varphi}_1 + C^{(m+1)} \varphi_1 \bar{\varphi}_{l+1} + D^{(m+1)} \varphi_{l+1} \bar{\varphi}_{l+1}] dx', \quad (\text{A7})$$

$$a^{(n+1)} = (\omega F)^{-1} (\Phi_1' B^{(n+1)} - \Phi_2' C^{(n+1)}), \quad (\text{A8})$$

$$b^{(n+1)} = -(\omega F)^{-1} (\Phi_1' A^{(n+1)} + \Phi_2' D^{(n+1)}),$$

$$c^{(n+1)} = (\omega F)^{-1} (\Phi_1' D^{(n+1)} + \Phi_2' A^{(n+1)}),$$

$$d^{(n+1)} = -(\omega F)^{-1} (\Phi_1' C^{(n+1)} - \Phi_2' B^{(n+1)}),$$

$$A^{(n+1)} = -\left(\frac{da^{(n)}}{dx} + T_+ a^{(n)}\right), \quad C^{(n+1)} = -\left(\frac{dc^{(n)}}{dx} + T_- c^{(n)}\right), \quad (\text{A9})$$

$$B^{(n+1)} = -\left(\frac{db^{(n)}}{dx} - T_- b^{(n)}\right), \quad D^{(n+1)} = -\left(\frac{dd^{(n)}}{dx} - T_+ d^{(n)}\right),$$

$$T_{\pm} = \frac{l+1}{\Phi_1} \Phi_1' \pm \frac{l+1}{\Phi_2} \Phi_2', \quad (\text{A10})$$

where the integral in the rhs of (A7) is the remainder of order m of the development of I into successive approximations; an overall factor $1/\omega^{m+1}$ can be extracted from it.

The question is left whether the integrals of type (A1) are convergent in the case of interest. To this aim some observations and assumptions, bearing on the structure of Φ_1 , Φ_2 , $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$, are necessary. We note that Φ_1' , Φ_2' , given by (A5) are respectively equal to $\exp(\lambda - \nu)/2$, $[\exp(\lambda - \nu)/2]/v_s$, where v_s is the velocity of sound; Φ_1' , Φ_2' , for a neutron star, are finite, different from zero and from one another, so that F , given by (A5) satisfies the inequality $|1/F| < C$.

Now let us make the following assumptions:

(1) The equation of state is such that Φ_1' , Φ_2' , λ , ν are analytical in r for $r=0$.

(2) $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are majorized by a constant C , for $0 \leq r \leq \bar{r}$, together with their derivatives with respect to r up to a certain order q .

(3) $A^{(0)}$ and $D^{(0)}$ are even functions of r for $r \rightarrow 0$, whereas $B^{(0)}$ and $C^{(0)}$ are odd.¹⁰

From (1) we conclude that T_{\pm} , as given by (A10), in the case under examination ($l'=l$), is an odd function of r and vanishes as r for $r \rightarrow 0$.

From (A8) and (A9), and from the above assumptions and results one proves by induction that $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, $A^{(n+1)}$, $B^{(n+1)}$, $C^{(n+1)}$, and $D^{(n+1)}$ are majorized by a constant C for $0 \leq r \leq \bar{r}$, $n \leq q$ and that $b^{(n)}$, $c^{(n)}$, $A^{(n+1)}$, and $D^{(n+1)}$ are even functions of r for $r \rightarrow 0$, whereas, $a^{(n)}$, $d^{(n)}$, $B^{(n+1)}$, and $C^{(n+1)}$ are odd.

Let us further consider the case $\bar{l}=l'$, $\Phi_1 = W_{\bar{r}}$, $\Phi_2 = x = W_s - W_s(r_0)$, $\bar{r} \leq r \leq r_0$, which is also involved in our problem; in this case the Bessel functions with index \bar{l} , $\bar{l}+1$ may diverge respectively as $x^{-\bar{l}}$, $x^{-(\bar{l}+1)}$ on the star surface. However, these are always multiplied by coefficients containing a factor x^{α} with $\alpha = \bar{l}+1$.

With reference to (A1) let us write such coefficients in the form:

$$A^{(0)} = f_1^{(0)} x^{\alpha}, \quad B^{(0)} = f_2^{(0)} x^{\alpha},$$

$$C^{(0)} = f_3^{(0)} x^{\alpha}, \quad D^{(0)} = f_4^{(0)} x^{\alpha}.$$

With reference to the primitive (A2) we set

$$a = \bar{a} x^{\alpha}, \quad b = \bar{b} x^{\alpha}, \quad c = \bar{c} x^{\alpha}, \quad d = \bar{d} x^{\alpha}. \quad (\text{A11})$$

In order to determine the lowest order approximation $\bar{a}^{(0)}$, $\bar{b}^{(0)}$, $\bar{c}^{(0)}$, and $\bar{d}^{(0)}$, we formally write \bar{a} , \bar{b} , \bar{c} , and \bar{d} in the form

$$\bar{a} = \sum_n \bar{a}^{(n)}, \quad \bar{b} = \sum_n \bar{b}^{(n)}, \quad (\text{A12})$$

$$\bar{c} = \sum_n \bar{c}^{(n)}, \quad \bar{d} = \sum_n \bar{d}^{(n)}.$$

Let us further replace (A11) and (A12) into the derivative with respect to x of (A2), and equate the coefficients of φ_{l+j} , $\varphi_{\bar{l}+j_1}$ ($j, j_1 = 0, 1$) relative to the largest power of ω in such a derivative with the analogous coefficients in the integrand of (A1).

In this way we obtain:

$$\bar{a}^{(0)} = \frac{v_s f_2^{(0)} - f_3^{(0)}}{\omega F}, \quad \bar{b}^{(0)} = -\frac{f_4^{(0)} + v_s f_1^{(0)}}{\omega F}, \quad (\text{A13})$$

$$\bar{c}^{(0)} = \frac{f_1^{(0)} + v_s f_4^{(0)}}{\omega F}, \quad \bar{d}^{(0)} = \frac{f_2^{(0)} - v_s f_3^{(0)}}{\omega F}.$$

Then the integral I can be written as

$$(\bar{a}^{(0)} \varphi_1 \bar{\varphi}_1 + \bar{b}^{(0)} \varphi_{l+1} \bar{\varphi}_1 + \bar{c}^{(0)} \varphi_1 \bar{\varphi}_{l+1} + \bar{d}^{(0)} \varphi_{l+1} \bar{\varphi}_{l+1}) x^{\alpha} + \int_x^x [x^{\alpha} (f_1^{(1)} \varphi_1 \bar{\varphi}_1 + f_2^{(1)} \varphi_{l+1} \bar{\varphi}_1 + f_3^{(1)} \varphi_1 \bar{\varphi}_{l+1} + f_4^{(1)} \varphi_{l+1} \bar{\varphi}_{l+1})]_x' dx', \quad (\text{A14})$$

where:

$$f_1^{(1)} = -\frac{1}{\omega} \left[\frac{v_s f_2^{(0)} - f_3^{(0)}}{F} \left(\frac{l+1}{W_{\bar{r}}} v_s + 2 \frac{\bar{l}+1}{x} \right) + \frac{d}{dx} \left(\frac{v_s f_2^{(0)} - f_3^{(0)}}{F} \right) \right],$$

$$f_2^{(1)} = \frac{1}{\omega} \left[\frac{f_4^{(0)} + v_s f_1^{(0)}}{F} \left(2 \frac{\bar{l}+1}{x} - \frac{l+1}{W_{\bar{r}}} v_s \right) + \frac{d}{dx} \left(\frac{f_4^{(0)} + v_s f_1^{(0)}}{F} \right) \right],$$

$$f_3^{(1)} = -\frac{1}{\omega} \left[\frac{l+1}{W_{\bar{r}}} v_s \frac{f_1^{(0)} + v_s f_4^{(0)}}{F} + \frac{d}{dx} \left(\frac{f_1^{(0)} + v_s f_4^{(0)}}{F} \right) \right],$$

$$f_4^{(1)} = -\frac{1}{\omega} \left[\frac{l+1}{W_{\bar{r}}} v_s \frac{v_s f_3^{(0)} - f_2^{(0)}}{F} + \frac{d}{dx} \left(\frac{v_s f_3^{(0)} - f_2^{(0)}}{F} \right) \right]. \quad (\text{A15})$$

The integral in the rhs of (A14) belongs to the same type as (A1); however, its coefficients, compared to

those of (A1), contain an additional factor $1/\omega$; we can thus set up a method of successive approximations for I for large values of $|\omega|$ by treating such an integral in a way similar to the previous one, and so on. The m th approximation reads

$$I = \sum_{n=0}^m [x^\alpha (\bar{a}^{(n)} \varphi_i \bar{\varphi}_i + \bar{b}^{(n)} \varphi_{i+1} \bar{\varphi}_i + \bar{c}^{(n)} \varphi_i \bar{\varphi}_{i+1} + \bar{d}^{(n)} \varphi_{i+1} \bar{\varphi}_{i+1})]_x^\alpha + \int_x^\alpha [x^\alpha (f_1^{(m+1)} \varphi_i \bar{\varphi}_i + f_2^{(m+1)} \varphi_{i+1} \bar{\varphi}_i + f_3^{(m+1)} \varphi_i \bar{\varphi}_{i+1} + f_4^{(m+1)} \varphi_{i+1} \bar{\varphi}_{i+1})]_{x'} dx', \quad (\text{A16})$$

where $f_k^{(m+1)}$ are related to $f_j^{(m)}$ ($k, j = 1, 2, 3, 4$) by the same relationships as those between $f_k^{(1)}$ and $f_j^{(0)}$, namely (A15); $\bar{a}^{(n)}$, $\bar{b}^{(n)}$, $\bar{c}^{(n)}$, and $\bar{d}^{(n)}$ are formally obtained from (A13) with the substitution of the index (0) with the index (n). Also in this case it must be verified that the successive approximations and their remainders are finite in the range of interest $\bar{r} \leq r \leq r_0$.

To this aim let us assume that:

- (4) $f_k^{(0)}$ are majorized by a constant C together with their derivatives up to a certain order q .
- (5) $f_1^{(0)}$ and $f_2^{(0)}$ behave like even functions of x in the limit $x \rightarrow 0$, whereas $f_3^{(0)}$ and $f_4^{(0)}$ behave like odd functions in the same limit.
- (6) $f_k^{(0)}$ are analytical in r in a certain neighborhood of $r = r_0$.¹¹

It easily follows by induction from (A13) and (A15) that $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, and $f_k^{(n+1)}$ are majorized by a constant C for $n \leq q$; in addition $f_1^{(n+1)}$, $f_2^{(n+1)}$, $c^{(n)}$, and $d^{(n)}$ behave like even function of x for $x \rightarrow 0$, whereas $f_3^{(n+1)}$, $f_4^{(n+1)}$, $a^{(n)}$, and $b^{(n)}$ behave like odd functions in the same limit for $n \leq q$.

Let us finally give a similar approach for integrals of type (A1) with $\Phi_1 = \Phi_2$; for the purpose of the present paper it will be enough to consider the case $l = l'$. Since the coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are arbitrary, we assume the variable x to coincide with $\Phi_1 = \Phi_2$.

First of all, integrating the last term of (A1) by parts we obtain, by means of (A3),

$$\int_x^\alpha D^{(0)} \varphi_{i+1} \bar{\varphi}_{i+1} dx' = \frac{1}{\omega} \int_x^\alpha \frac{dD^{(0)}}{dx} \varphi_i \bar{\varphi}_{i+1} dx' + \int_x^\alpha D^{(0)} \varphi_i \bar{\varphi}_i dx' - \frac{1}{\omega} D^{(0)} \varphi_i \bar{\varphi}_{i+1}, \quad (\text{A17})$$

moreover, recalling that, owing to a property of Bessel functions, the expression $\varphi_i \bar{\varphi}_{i+1} - \bar{\varphi}_i \varphi_{i+1}$ is a constant, again with the help of (A3), one obtains by further partial integrations

$$\begin{aligned} & \int_x^\alpha (f_1 \varphi_{i+1} \bar{\varphi}_i + f_2 \varphi_i \bar{\varphi}_{i+1}) dx' \\ &= \frac{1}{\omega} \int_x^\alpha \left[\frac{l+1}{x} (f_1 + f_2) + \frac{1}{2} \frac{d}{dx} (f_1 + f_2) \right]_{x'} \varphi_i \bar{\varphi}_i dx' \\ &+ \frac{1}{2} (\varphi_{i+1} \bar{\varphi}_i - \varphi_i \bar{\varphi}_{i+1}) \int_0^x (f_1 - f_2) dx' - \frac{1}{2\omega} (f_1 + f_2) \varphi_i \bar{\varphi}_i, \end{aligned} \quad (\text{A18})$$

where f_1 and f_2 are slowly varying functions.

Using up the above relations for the primitive P of (A1) we get

$$P = \int_x^\alpha f^{(0)} \varphi_i \bar{\varphi}_i dx' + \frac{1}{2} (\varphi_{i+1} \bar{\varphi}_i - \varphi_i \bar{\varphi}_{i+1}) \times \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right) dx' - \frac{1}{\omega} D^{(0)} \varphi_i \bar{\varphi}_{i+1} - \frac{1}{2\omega} \left(B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right) \varphi_i \bar{\varphi}_i, \quad (\text{A19})$$

$$f^{(0)} = A^{(0)} + D^{(0)} + \left[\frac{l+1}{\omega x} + \frac{1}{2\omega} \frac{d}{dx} \right] \times \left(B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right). \quad (\text{A20})$$

Now using (A3) one can verify the equality (by derivation of both sides)

$$\begin{aligned} & \int_x^\alpha f_i^{(0)} \varphi_i \bar{\varphi}_i dx' \\ &= \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \\ &+ \frac{1}{2} \int_0^x f^{(0)} dx' (\varphi_i \varphi_i + \varphi_{i+1} \varphi_{i+1}) - \frac{1}{4\omega} \int_x^\alpha \left[\frac{d}{dx} \left(f^{(0)} - \frac{2(l+1)}{x'} \int_0^x f^{(0)} dx'' \right) (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \right]_{x'} dx'. \end{aligned} \quad (\text{A21})$$

Then from (A19) and the above equality, one obtains

$$I = [a^{(0)} \varphi_i \bar{\varphi}_i + b^{(0)} \varphi_{i+1} \bar{\varphi}_i + c^{(0)} \varphi_i \bar{\varphi}_{i+1} + d^{(0)} \varphi_{i+1} \bar{\varphi}_{i+1}]_a^\alpha - \frac{1}{4\omega} \int_a^\alpha \left[\frac{d}{dx} \left(f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx'' \right) (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \right]_{x'} dx', \quad (\text{A22})$$

$$a^{(0)} = \frac{1}{2} \int_0^x f^{(0)} dx' - \frac{1}{2\omega} \left[B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right],$$

$$b^{(0)} = \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] + \frac{1}{2} \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right)_{x'} dx', \quad (\text{A23})$$

$$c^{(0)} = \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] - \frac{1}{2} \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right)_{x'} dx' - \frac{1}{\omega} D^{(0)},$$

$$d^{(0)} = \frac{1}{2} \int_0^x f^{(0)} dx'.$$

The integral in the rhs of (A22) belongs to the original type (A1); however its coefficients exhibit (at least) a factor $1/\omega$ in comparison with the original coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$.

A similar approach can be applied to this integral, and so on, for the successive approximations. The m th approximation is formally written as (A7) in which

$$A^{(n+1)} = D^{(n+1)} = 0,$$

$$B^{(n+1)} = C^{(n+1)} = -\frac{1}{4\omega} \frac{d}{dx} \left[f^{(n)} - \frac{2(l+1)}{x} \int_0^x f^{(n)} dx' \right], \quad (\text{A24})$$

and $a^{(n+1)}$, $b^{(n+1)}$, $c^{(n+1)}$, and $d^{(n+1)}$ are related to $f^{(n+1)}$ and $B^{(n+1)}$ by the same relationships (A23) which connect $a^{(0)}$, $b^{(0)}$, $c^{(0)}$, and $d^{(0)}$ to $f^{(0)}$, $B^{(0)}$, where formally one sets $C^{(0)} = B^{(0)}$, $D^{(0)} = 0$.

Once again it must be verified that the successive approximations are convergent for $x \rightarrow 0$ in the cases of interest. To this aim we make the following assumptions analogous to (4), (5), and (6).

(7) $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are majorized by a constant C together with their derivatives up to a certain order q , respectively, in the intervals $0 \leq x \leq x(\bar{r})$ when $x = W_g$ or W_s and $0 \geq x \geq W_s(\bar{r}) - W_s(r_0)$ when $x = W_s - W_s(r_0)$.

(8) $A^{(0)}$ and $D^{(0)}$ behave as even functions for $x \rightarrow 0$, whereas $B^{(0)}$ and $C^{(0)}$ behave as odd functions in the same limit.

(9) The coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are analytical in a neighborhood of $r=0$, or $r=r_0$ according to whether the first or the second interval is considered.¹¹

Then one easily proves by induction that $f^{(n)}$, $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, and $B^{(n+1)} = C^{(n+1)}$ for $n \leq q$ are majorized by a constant C in the intervals considered in (6),

according to the specifications made there; in addition $b^{(n)}$, $c^{(n)}$, and $f^{(n)}$ have an even character for $x \rightarrow 0$, where $a^{(n)}$, $d^{(n)}$, and $B^{(n+1)} = C^{(n+1)}$ have an odd character in the same limit.

¹P. Cazzola, L. Lucaroni, and R. Semenzato, *J. Math. Phys.* **19**, 237 (1978).

²For the definition of W_s , W_g see (I.3.19) [paper I above, Eq. (3.19)].

³P. Cazzola and L. Lucaroni, *Phys. Rev. D* **6**, 950 (1972).

⁴R. G. Newton, *J. Math. Phys.* **1**, 319 (1960).

⁵T. Regge, *Nuovo Cimento* **9**, 295 (1958).

⁶Here and in the following C or C_1, C_2, \dots denote positive ω -independent constants.

⁷One easily verifies that the normalization for u defined in (3) in the limit $r \rightarrow 0$ coincides with the one given by (5.1) and (5.3).

⁸Equation (6.7) holds with the exception of those values of ω in the real axis for which $\eta_s^{(0)}(r_0)$ vanishes; but these never coincide with the eigenfrequencies in which we are interested.

⁹L. Battiston, P. Cazzola, and L. Lucaroni, *Nuovo Cimento B* **3**, 295 (1971).

¹⁰We note that 2) can be verified by inspection, whereas Φ'_1 , Φ'_2 , λ , ν are even functions of r in a neighborhood of $r=0$ as a consequence of the equilibrium equations. 3) follows from the above statement and from the definite parity character of the coefficients of the coupled equations (I.2.10) and (I.2.23).

¹¹For the integrals involved in our problem 4), 7) can be verified by inspection. As regards 5), 6), 8), 9) it is evident that, even if they do not hold, the above formulas are valid up to a certain order of approximation such that, at any step, the coefficients of the cited byproducts in the remainders are finite. Since in the calculation of the integrals involved in Secs. 5 and 7 it is sufficient to consider the lowest order approximations, we can see by inspection that the above conditions are satisfied. The remainders are then majorized according to standard procedures developed in paper I or in Sec. 3, and are shown to be negligible.

Asymptotic eigenfrequency distribution for even-parity perturbations of hot perfect-fluid relativistic neutron stars^{a)}

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Making two assumptions regarding the analytical continuation of the external solution to the region $\text{Im}\omega < 0$, we give the asymptotic distribution for $\omega \rightarrow \infty$ of the eigenfrequencies of a hot perfect fluid relativistic neutron star. It results that the real parts of the complex eigenfrequencies grow as the integers, while their imaginary parts grow as $\ln|\omega_r|$ with coefficients depending inversely on the "optical path" of the uncoupled gravitational waves through the star.

1. INTRODUCTION

In a previous paper,¹ hereafter referred to as I, we set up two systems of integral equations for even parity perturbations of perfect fluid neutron stars; their solutions describe coupled sound and gravitational waves of given frequency ω , in the framework of a single multipole of order $l \geq 2$.

The two solutions of such equations are linearly combined in order to obtain the physical solution (up to a multiplicative constant) by the requirement that the Lagrangian variation of the pressure vanishes on the star surface.

In that paper we gave an argument suggesting that the coupling between the two kinds of waves becomes weaker and weaker for $\omega \rightarrow \infty$, whereas the successive iterations furnish successive approximations to the solutions in such a limit.

In the present paper, we will prove this statement and explicitly give the physically significant internal solution for $\omega \rightarrow \infty$.

The linear combination expressing the physical solution u for the gravitational amplitude contains terms whose absolute value is proportional to $\exp|\text{Im}\omega|W_s$.² However, as a result of cancellations, the physical solution can be rewritten as a linear combination of terms whose order of magnitude is less than or equal to $\exp|\text{Im}\omega|W_g \leq \exp|\text{Im}\omega|W_s$.² A part of this paper is devoted to the proof that such cancellations occur at any order in the successive iterations. To this aim we define here new "zero order iterations" which are given by systems of integral equations including gravitational and matter field "self-interactions." In this way new integral equations, which take into account only the coupling between sound and gravitational waves, are constructed and from them the physically significant

solution is derived. The advantage of this new method lies in the fact that it makes it easier to prove the aforementioned cancellations. After this proof is worked out the computation of the dominant terms in u which do not cancel turns out to be straightforward.

The significant internal solution allows us to determine the asymptotic distribution of the eigenfrequencies in the upper ω plane, provided two reasonable assumptions (whose validity will be the object of a subsequent paper) is made on the analytical continuation of the external solution in the lower ω plane.

In fact, the knowledge of such continuation is necessary since the eigenfrequencies coincide with the zeroes of $W(-\omega)$, where W is the Wronskian function constructed with the external and gravitational solution at the star surface.³ In the framework of the cited assumptions it is found that, in the region $\text{Im}\omega > 0$, the distribution turns out to be very similar to that of the poles of the S matrix for the scattering of a particle in a potential field in quantum mechanics, when the potential is truncated or decreases at least more than any exponential.^{4,5}

The plan of the paper is the following:

In Sec. 2 we give the modified integral equations for the internal solutions, whose zero order iterations take into account the sound and gravitational "self-coupling."

In Sec. 3 majorizations for such zero order iterations are given.

In Sec. 4 the amplitudes which are needed in order to construct the physical internal solution are suitably majorized.

In Sec. 5 a representation of the internal physical solution, suitable for the subsequent majorizations, is given.

In Sec. 6 it is showed that the physical internal solution, for $\omega \rightarrow \infty$, is a combination of terms whose order of magnitude is less than or equal to $\exp|\text{Im}\omega|W_g$.

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In Sec. 7 the Wronskian function is constructed and its leading terms for $\omega \rightarrow \infty$ are calculated; the asymptotic distribution of the eigenfrequencies is finally derived.

In the Appendix we set up a method of successive approximations for integrals appearing in Sec. 7.

2. MODIFIED INTEGRAL EQUATIONS FOR THE INTERNAL SOLUTIONS

The symbols which are not defined in the present context are defined in paper I.

Let us consider the following equation in $U^{(0)}$,

$$[O_1 - V_{11}]U^{(0)} = 0, \quad (2.1)$$

where the linear differential operator $O_1 - V_{11}$ is the one acting on the variable u in (I. 2. 10). Then let us introduce the integral equations [whose solutions obey (2. 1)]

$$U_g^{(0)} = u_g^{(0)} + \int_0^r g_1(r, r')(V_{11}U_g^{(0)})_{r'} dr', \quad (2.2)$$

$$U_\sigma^{(0)} = u_\sigma^{(0)} + \int_{r_0}^r g_1(r, r')(V_{11}U_\sigma^{(0)})_{r'} dr', \quad (2.3)$$

$$u_\sigma^{(0)} = \phi_g \bar{h}_i^{(\sigma)}(x_g), \quad \sigma = \text{sign}(\text{Im}\omega), \quad (2.4)$$

where ϕ_g is given by (I. 3. 20) and $x_g = \omega W_g$, W_g being given by (I. 3. 6); $\bar{h}_i^{(\sigma)}(x_g)$, defined by (I. 3. 22), satisfies the inequality⁶

$$|\bar{h}_i^{(\sigma)}(x_g)| < C \exp(-|\text{Im}\omega| W_g) [L(|x_g|)]^{-1}, \quad (2.5)$$

where $L(x) = x/(1+x)$.

$U_g^{(0)}$, $U_\sigma^{(0)}$ are respectively regular and irregular for $r=0$.

Similarly consider the following equation in $H^{(0)}$,

$$[O_2 - V_{22}]H^{(0)} = 0, \quad (2.6)$$

where the linear differential operator $O_2 - V_{22}$ is the one acting on the variable η in (I. 2. 23).

Let us introduce the integral equations [whose solutions obey (2. 6)]

$$H_s^{(0)} = \eta_s^{(0)} + \int_0^r g_2(r, r')(V_{22}H_s^{(0)})_{r'} dr', \quad (2.7)$$

$$H_\sigma = \eta_\sigma^{(0)} + \int_{r_0}^r g_2(r, r')(V_{22}H_\sigma^{(0)})_{r'} dr', \quad (2.8)$$

$$\eta_\sigma^{(0)} = \phi_s [\vartheta(r - \bar{r}) \bar{h}_i^{(\sigma)}(X) \exp[-|\text{Im}\omega| W_0] + \vartheta(\bar{r} - r) (c_+ \bar{h}_i^{(\sigma)}(x_s) + c_- \bar{h}_i^{(-\sigma)}(x_s))], \quad (2.9)$$

where ϕ_s, X, W_s, W_0 are given respectively by (I. 3. 21), (I. A13), (I. 3. 8), and $x_s = \omega W_s$; c_+, c_- are determined by imposing the continuity of $\eta_\sigma^{(0)}$ and of its derivative with respect to r at the junction point \bar{r} . One verifies that

$$|\eta_\sigma^{(0)}/\phi_s| < C \exp(-|\text{Im}\omega| W_s) \times \{\theta(\bar{r} - r) [L(|x_s|)]^{-1} + \theta(r - \bar{r}) [L(|X|)]^{-1}\}. \quad (2.10)$$

$H_s^{(0)}$ and $H_\sigma^{(0)}$ are respectively regular and irregular for $r=0$.

In comparison with paper I, $U_g^{(0)}$ and $H_s^{(0)}$ furnish new zero-order iterations for solutions of the "gravitational" and "matter field" type instead of $u_g^{(0)}$, $\eta_s^{(0)}$.

In principle they account exactly for the self-interaction terms $V_{11}u$ and $V_{22}\eta$ appearing in (I. 3. 3) and (I. 3. 4).

To be more definite, we can construct new regular solutions of the original Eqs. (I. 2. 10) and (I. 2. 23) determined by the following systems of integral equations [to be compared with (I. 3. 26) and (I. 3. 27)],

$$U_g = U_g^{(0)} + \int_0^r G_1(r, r')(V_{12}H_g)_{r'} dr', \quad (2.11)$$

$$H_g = \int_0^r G_2(r, r')(V_{21}U_g)_{r'} dr',$$

$$U_s = \int_0^r G_1(r, r')(V_{12}H_s)_{r'} dr', \quad (2.12)$$

$$H_s = H_s^{(0)} + \int_0^r G_2(r, r')(V_{21}U_s)_{r'} dr',$$

$$G_1(r, r') = -\frac{U_g^{(0)}(r)U_\sigma^{(0)}(r') - U_\sigma^{(0)}(r)U_g^{(0)}(r')}{[W(U_g^{(0)}; U_\sigma^{(0)})]_{r'}}, \quad (2.13)$$

$$G_2(r, r') = -\frac{H_s^{(0)}(r)H_\sigma^{(0)}(r') - H_\sigma^{(0)}(r)H_s^{(0)}(r')}{[W(H_s^{(0)}; H_\sigma^{(0)})]_{r'}}, \quad (2.14)$$

where $W(\psi_1, \psi_2)$ is the Wronskian constructed with ψ_1 and ψ_2 .

3. MAJORIZATION OF $U_g^{(0)}$, $U_\sigma^{(0)}$, $H_s^{(0)}$, $H_\sigma^{(0)}$

In the following, frequent use will be made of inequalities relative to the functions ϕ_g, ϕ_s implied in the definitions of $u_g^{(0)}$, $u_\sigma^{(0)}$, $\eta_s^{(0)}$, $\eta_\sigma^{(0)}$. These hold for ω large enough and are easily verified by inspection,

$$C_1 < r\phi_g < C_2, \quad (3.1)$$

$$C_1 < r(\rho + p)^{-1/2} v_s^{-1/2} \phi_s < C_2. \quad (3.2)$$

Successive iterations can be given for the Eqs. (2. 2), (2. 3)

$$U_g^{(0, n+1)} = \int_0^r g_1(r, r')(V_{11}U_g^{(0, n)})_{r'} dr', \quad (3.3)$$

$$U_\sigma^{(0, n+1)} = \int_{r_0}^r g_1(r, r')(V_{11}U_\sigma^{(0, n)})_{r'} dr', \quad (3.4)$$

$$U_g^{(0, 0)} = u_g^{(0)}, \quad U_\sigma^{(0, 0)} = u_\sigma^{(0)}. \quad (3.5)$$

Let us set

$$U_g^{(0)} = \bar{U}_g^{(0)} r^{-1} [L(|x_g|)]^{1+1} \exp[|\text{Im}\omega| W_g], \quad (3.6a)$$

$$\bar{g}_1(r, r') = g_1(r, r')(r/r') [L(|x_g|)]^{-(1+1)} \times \exp[|\text{Im}\omega| (W_g' - W_g)], \quad (3.6b)$$

$$\bar{V}_{11} = V_{11} \exp[(\nu - \lambda)/2] v_s [L(|x_g|)]^{1+1}. \quad (3.6c)$$

From (3. 3), (3. 5), and (3. 6) one obtains

$$\bar{U}_g^{(0, n)} = \int_0^W \bar{g}_1(r, r_1) \bar{V}_{11}(r_1) dW_{s1} \int_0^{W_{s1}} \bar{g}_1(r_1, r_2) \bar{V}_{11}(r_2) dW_{s2} \dots \int_0^{W_{sn-1}} \bar{g}_1(r_{n-1}, r_n) \bar{V}_{11}(r_n) \bar{U}_g^{(0, 0)} dW_{sn}. \quad (3.7)$$

Furthermore by inspection one can see that $\bar{U}_g^{(0, 0)} = \bar{u}_g^{(0)}$, $\bar{g}_1 \bar{V}_{11} = \bar{g}_1' \bar{V}_{11}'$, where $\bar{u}_g^{(0)}$, \bar{V}_{11}' , \bar{g}_1' are defined by (I. 4. 4), (I. 4. 7), (I. 4. 9). Then from (I. 4. 13), (I. 4. 14) for $r' \leq r$ we obtain

$$|\bar{g}_1(r, r') \bar{V}_{11}'(r')| < \frac{C}{|\omega|}, \quad |\bar{U}_g^{(0, 0)}| < C. \quad (3.8)$$

From the above inequalities and (3.7) we get

$$|\bar{U}_\varepsilon^{(0,n)}| < \frac{C^{n+1}W_s^m}{|\omega|^{n+1}} \quad (3.9)$$

and then from (3.6a), by summation of all iterations,

$$|U_\varepsilon^{(0)}| < Cr^{-1}[L(|x_\varepsilon|)]^{l+1} \exp[|\operatorname{Im}\omega|W_\varepsilon]. \quad (3.10)$$

In a similar way, introducing

$$U_\sigma^{(0)} = \hat{U}_\sigma^{(0)} r^{-1} [L(|x_\sigma|)]^{-l} \exp(-|\operatorname{Im}\omega|W_\sigma), \quad (3.11a)$$

$$\hat{g}_1(r, r') = g_1(r, r') [L(|x_\sigma|)]^l \exp[|\operatorname{Im}\omega|(W_\sigma - W'_\sigma)], \quad (3.11b)$$

$$\hat{V}_{11} = V_{11} \exp[(\nu - \lambda)/2] v_s [L(|x_\sigma|)]^{-l}, \quad (3.11c)$$

one can see by inspection that $\hat{g}_1 \hat{V}_{11} = \tilde{g}_1 \tilde{V}_{11} \exp[2|\operatorname{Im}\omega| \times (W_\sigma - W'_\sigma)]$,

so that, owing to (I. 4.13), one obtains

$$|\hat{g}_1(r, r') \hat{V}_{11}(r')| < \frac{C}{|\omega|}, \quad r \leq r', \quad (3.12)$$

and taking into account (2.5), (3.1), and (3.11a) one obtains

$$|\hat{U}_\sigma^{(0,0)}| < C. \quad (3.13)$$

Then, with the help of the above inequality, together with (3.4) and (3.12), with a procedure quite similar to that outlined for $U_\varepsilon^{(0)}$, we get

$$|U_\sigma^{(0)}| < Cr^{-1}[L(|x_\sigma|)]^{-l} \exp(-|\operatorname{Im}\omega|W_\sigma). \quad (3.14)$$

In an analogous way the successive iterations of (2.7) and (2.8) read

$$H_s^{(0,n+1)} = \int_0^r g_2(r, r') (V_{22} H_s^{(0,n)})_{r'} dr', \quad (3.15)$$

$$H_\sigma^{(0,n+1)} = \int_0^r g_2(r, r') (V_{22} H_\sigma^{(0,n)})_{r'} dr', \quad (3.16)$$

$$H_s^{(0,0)} = \eta_s^{(0)}, \quad H_\sigma^{(0,0)} = \eta_\sigma^{(0)}. \quad (3.17)$$

Then let us introduce

$$H_s^{(0)} = \bar{H}_s^{(0)} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \quad (3.18a)$$

$$\begin{aligned} \bar{g}_2(r, r') = g_2(r, r') \frac{r}{r'} \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|(W'_s - W_s)], \end{aligned} \quad (3.18b)$$

$$\bar{V}_{22} = V_{22} e^{(\nu - \lambda)/2} v_s \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \quad (3.18c)$$

and

$$H_\sigma^{(0)} = \hat{H}_\sigma^{(0)} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l} + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp(-|\operatorname{Im}\omega|W_\sigma), \quad (3.19a)$$

$$\begin{aligned} \hat{g}_2(r, r') = g_2(r, r') \frac{r}{r'} \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \{ \theta(\bar{r} - r) [L(|x_s|)]^l \\ + \theta(r - \bar{r}) [L(|X|)]^l \} \exp[|\operatorname{Im}\omega|(W_s - W'_\sigma)], \end{aligned} \quad (3.19b)$$

$$\begin{aligned} \hat{V}_{22} = V_{22} \exp[(\nu - \lambda)/2] v_s \{ [L(|x_s|)]^{-l} \theta(\bar{r} - r) \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \}. \end{aligned} \quad (3.19c)$$

Now one can verify that $\bar{H}_s^{(0,0)} = \tilde{\eta}_s^{(0)}$, $\bar{g}_2 \bar{V}_{22} = \tilde{g}_2 \tilde{V}_{22}$, and

$$\tilde{g}_2 \hat{V}_{22} = \tilde{g}_2 \tilde{V}_{22} \exp[2|\operatorname{Im}\omega|(W_s - W'_\sigma)],$$

where $\tilde{\eta}_s^{(0)}$, \tilde{V}_{22} , and \tilde{g}_2 are defined by (I. 4.5), (I. 4.8), and (I. 4.10). Then from (I. 4.13) and (I. 4.14) it follows that:

$$|\bar{g}_2(r, r') \bar{V}_{22}(r')| < \frac{C}{|\omega|}, \quad r' \leq r, \quad (3.20)$$

$$|\hat{g}_2(r, r') \hat{V}_{22}(r')| < \frac{C}{|\omega|}, \quad r \leq r', \quad (3.21)$$

$$|\bar{H}_s^{(0,0)}| < C. \quad (3.22)$$

In addition, an inequality similar to (3.13) is easily derived,

$$|\hat{H}_\sigma^{(0,0)}| < C. \quad (3.23)$$

Finally, with a procedure similar to that outlined in order to obtain (3.10) and (3.14), we get

$$\begin{aligned} |H_s^{(0)}| < Cr^{-1} (W_0 - W_s)^l \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \end{aligned} \quad (3.24)$$

$$\begin{aligned} |H_\sigma^{(0)}| < Cr^{-1} (W_0 - W_s)^l \{ \theta(\bar{r} - r) [L(|x_s|)]^{-l} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp(-|\operatorname{Im}\omega|W_s). \end{aligned} \quad (3.25)$$

4. MAJORIZATIONS OF H_g, H_s

A program parallel to that of Sec. 4 of paper I can now be developed for the coupled integral equations (2.11) and (2.12); however, in the present context, we are interested only in the amplitudes H . Let us set

$$\begin{aligned} H = \bar{H} r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\ + \theta(r - \bar{r}) [L(|X|)]^{-l} \} \exp[|\operatorname{Im}\omega|W_s], \end{aligned} \quad (4.1)$$

$$U = \bar{U} r^{-1} [L(|x_s|)]^{l+1} \exp[|\operatorname{Im}\omega|W_s], \quad (4.2)$$

$$\bar{G}_1(r, r') = G_1(r, r') \frac{r}{r'} [L(|x_s|)]^{-l+1} \exp[|\operatorname{Im}\omega|(W'_s - W_s)], \quad (4.3)$$

$$\begin{aligned} \tilde{G}_2(r, r') = G_2(r, r') \frac{r}{r'} \exp[|\operatorname{Im}\omega|(W'_s - W_s)] \frac{[(\rho + p)^{1/2} v_s^{1/2}]^{r'}}{(\rho + p)^{1/2} v_s^{1/2}} \\ \times \{ [L(|x_s|)]^{-l+1} \theta(\bar{r} - r) + \theta(r - \bar{r}) [L(|X|)]^{-l} \}. \end{aligned} \quad (4.4)$$

We want to prove now that

$$|\tilde{G}_1(r, r') \tilde{V}_{12}(r')| < \frac{C}{|\omega|^3}, \quad (4.5)$$

$$|\tilde{G}_2(r, r') \tilde{V}_{21}(r')| < \frac{C}{|\omega|^3}, \quad (4.6)$$

where $\tilde{V}_{12}, \tilde{V}_{21}$ are defined by (I. 4.7), (I. 4.8).

In order to do this it is necessary to give suitable majorizations of $G_1(r, r')$ and $G_2(r, r')$, given by (2.13) and (2.14), and therefore, among other things, to assign minorizations of the Wronskians appearing in them.

From (2.2) and (2.3) one gets

$$\begin{aligned}
 & W(U_g^{(0)}; U_s^{(0)}) \\
 &= W(u_g^{(0)}; u_s^{(0)}) \left[1 + \omega^{-1} \int_0^r \frac{u_s^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \right. \\
 &\quad - \omega^{-1} \int_0^r \frac{u_g^{(0)} V_{11} U_s^{(0)}}{\phi_s^2 \exp[(\lambda - \nu)/2]} dr' \\
 &\quad - \omega^{-2} \int_0^r \frac{u_s^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \int_{r_0}^r \frac{u_g^{(0)} V_{11} U_s^{(0)}}{\phi_s^2 \exp[(\lambda - \nu)/2]} dr' \\
 &\quad \left. + \omega^{-2} \int_0^r \frac{u_g^{(0)} V_{11} U_s^{(0)}}{\phi_s^2 \exp[(\lambda - \nu)/2]} dr' \int_{r_0}^r \frac{u_s^{(0)} V_{11} U_g^{(0)}}{\phi_g^2 \exp[(\lambda - \nu)/2]} dr' \right]. \quad (4.7)
 \end{aligned}$$

Taking into account the inequality $|V_{11}| < C$, quoted in the appendix of paper I, and making use of (3.1), (3.6a), (3.8), (3.11a), (3.13), and (3.14) one obtains

$$|W(U_g^{(0)}; U_s^{(0)})| > Cr^{-2} |\omega|. \quad (4.8)$$

In a similar way one can minorize the Wronskian appearing in $G_2(r, r')$ making use of (3.2), (3.18a), (3.22), (3.19a), (3.23), (3.24), and (3.25) together with (I.3.15)

$$\begin{aligned}
 & W(H_s^{(0)}; H_g^{(0)}) W(\eta_s^{(0)}; \eta_g^{(0)}) \left(1 + \frac{Q}{\omega} \right) \\
 &= -\omega \phi_s^2 \frac{\exp(\lambda - \nu)/2}{v_s}, \quad |Q| < C, \quad (4.9)
 \end{aligned}$$

$$|W(H_s^{(0)}; H_g^{(0)})| > Cr^{-2}(\rho + p) |\omega|.$$

Taking into account that V_{21} and V_{12} , given by (I.3.11), are respectively proportional to $(\rho + p)\omega^{-4}$ and ω^{-2} , from (3.10), (3.14), (3.24), (3.25), (4.8), and (4.9), we straightforwardly get the inequalities (4.5) and (4.6).

Comparing (4.1), (4.2) respectively with (3.18a), (3.6a) we get by means of (3.24), (3.10),

$$|\tilde{H}_s^{(0)}| = |\bar{H}_s^{(0)}| < C, \quad (4.10)$$

$$\begin{aligned}
 |\tilde{U}_g^{(0)}| &= |\bar{U}_g^{(0)}| [L(|x_g|)/L(|x_s|)]^{l+1} \exp[|\operatorname{Im}\omega| (W_g - W_s)] \\
 &< C. \quad (4.11)
 \end{aligned}$$

Finally from (2.11), (2.12) together with (4.1), (4.2), one gets

$$\begin{aligned}
 \tilde{H}_g^{(n)} &= \frac{1 - (-1)^n}{2} \int_0^W \tilde{G}_2(r, r_1) \tilde{V}_{21}(r_1) dW_{s_1} \\
 &\quad \times \int_0^{W_{s_1}} \tilde{G}_1(r_1, r_2) \tilde{V}_{12}(r_2) dW_{s_2} \dots \\
 &\quad \int_0^{W_{s_{n-1}}} \tilde{G}_2(r_{n-1}, r_n) \tilde{V}_{21}(r_n) \tilde{U}_g^{(0)}(r_n) dW_{s_n}, \quad (4.12)
 \end{aligned}$$

$$\begin{aligned}
 \tilde{H}_s^{(n)} &= \frac{1 + (-1)^n}{2} \int_0^W \tilde{G}_2(r, r_1) \tilde{V}_{21}(r_1) dW_{s_1} \\
 &\quad \times \int_0^{W_{s_1}} \tilde{G}_1(r_1, r_2) \tilde{V}_{12}(r_2) dW_{s_2} \dots \\
 &\quad \int_0^{W_{s_{n-1}}} \tilde{G}_1(r_{n-1}, r_n) \tilde{V}_{12} \tilde{H}_s^{(0)}(r_n) dW_{s_n}. \quad (4.13)
 \end{aligned}$$

From these and from (4.5), (4.6), (4.10), and (4.11) it follows that

$$|\tilde{H}_g^{(n)}| < \frac{C^{n+1} W_s^m}{n! |\omega|^{4n+1}}, \quad (4.14)$$

$$|\tilde{H}_s^{(n)}| < \frac{C^{n+1} W_s^m}{n! |\omega|^{4n}}, \quad (4.15)$$

and then, in analogy with (I.4.16),

$$\begin{aligned}
 \left| \sum_{n=0}^{\infty} \left[\frac{H_g^{(n)}}{H_s^{(n)}} \right] \right| &< r^{-1} (\rho + p)^{1/2} v_s^{1/2} \{ \theta(\bar{r} - r) [L(|x_s|)]^{l+1} \\
 &\quad + [L(|X|)]^{-l} \theta(r - \bar{r}) \} \exp[|\operatorname{Im}\omega| W_s] \\
 &\quad \times \frac{C^{m+1} W_s^m}{m! |\omega|^m} \exp\left(\frac{CW_0}{|\omega|}\right). \quad (4.16)
 \end{aligned}$$

5. REPRESENTATION OF THE PHYSICAL SOLUTION

In analogy with (I.3.30), (I.3.31), and (I.3.32), the physical solution can be alternatively written as⁷

$$u = U_g + \mu_1 U_s, \quad (5.1)$$

$$\eta = H_g + \mu_1 H_s, \quad (5.2)$$

$$\mu_1 = -(H_g/H_s)_{r_0}; \quad (5.3)$$

it follows that

$$\begin{aligned}
 u &= (H_s(r_0) U_g - U_s H_g(r_0)) \frac{1}{H_s(r_0)} \\
 &= \frac{1}{H_s(r_0)} \sum_{n=0}^{\infty} \sum_{j=0}^n [H_s^{(j)}(r_0) U_g^{(n-j)} - U_s^{(j)} H_g^{(n-j)}(r_0)]. \quad (5.4)
 \end{aligned}$$

Now (4.12) and (4.13) imply the relations $H_g^{(2n)} = H_s^{(2n+1)} = 0$, which also lead to $U_g^{(2n+1)} = U_s^{(2n)} = 0$ by iteration of (2.11) and (2.12). Then we get

$$\begin{aligned}
 u &= \frac{1}{H_s(r_0)} \sum_{n=0}^{\infty} \left[\theta(2n-1) \left(\sum_{j=0}^{2n-1} H_s^{(j)}(r_0) U_g^{(2n-j)} \right) \right. \\
 &\quad \left. - \sum_{j=1}^{2n} U_s^{(j)} H_g^{(2n-j)}(r_0) \right] + H_s^{(2n)}(r_0) U_g^{(0)}. \quad (5.5)
 \end{aligned}$$

Introducing in (5.5) the iterations of (2.11) and (2.12) for U_g and U_s we further obtain

$$u = U_g^{(0)} + \sum_{n=1}^{\infty} S^{(n)}, \quad (5.6)$$

$$S^{(n)} = \frac{1}{H_s(r_0)} \int_0^r G_1(r, r') V_{12}(r') \Lambda^{(2n-1)}(r_0, r') dr', \quad (5.7)$$

$$\begin{aligned}
 \Lambda^{(n)}(r_0, r') &= \sum_{j=0}^{n-1} [H_s^{(2j)}(r_0) H_g^{(2n-2j-1)}(r') \\
 &\quad - H_s^{(2j)}(r') H_g^{(2n-2j-1)}(r_0)]. \quad (5.8)
 \end{aligned}$$

Now, as stated in Sec. 1, we want to show that u is proportional to $\exp|\operatorname{Im}\omega| W_g$ despite the fact that most of the terms appearing in it behave like $\exp|\operatorname{Im}\omega| W_s$. In order to do this a suitable representation of the expressions in the square brackets is necessary.

Let us define

$$k = - \int_0^r \frac{H_g^{(0)} V_{21} U_g^{(0)}}{W(H_s^{(0)}; H_g^{(0)})} dr', \quad (5.9)$$

$$I_1(r, r') = \frac{H_s^{(0)}(r) H_g^{(0)}(r') V_{21}(r')}{[W(H_s^{(0)}; H_g^{(0)})]_{r'}}, \quad (5.10)$$

$$I_2(r, r') = \frac{H_g^{(0)}(r) H_s^{(0)}(r') V_{21}(r')}{[W(H_s^{(0)}; H_g^{(0)})]_{r'}}, \quad (5.11)$$

$$f_1(r) = \int_r^{r_0} I_1(r, r') U_g^{(0)}(r') dr' + \int_0^r I_2(r, r') U_g^{(0)}(r') dr', \quad (5.12)$$

$$f_2(r) = \int_0^r G_1(r, r') (V_{12} f_1)_{r'} dr', \quad (5.13)$$

$$\dots \dots \dots f_{2n+1}(r) = \int_r^{r_0} I_1(r, r') f_{2n}(r') dr' + \int_0^r I_2(r, r') f_{2n}(r') dr', \quad (5.14)$$

$$f_{2n+2}(r) = \int_0^r G_1(r, r') (V_{12} f_{2n+1})_{r'} dr'. \quad (5.15)$$

From (5.9)–(5.12) we get

$$\int_0^r G_2(r, r') (V_{21} U_g^{(0)})_{r'} dr' = k H_s^{(0)} + f_1. \quad (5.16)$$

Then for the terms $H_s^{(2j)}(r_0) H_g^{(2n-2j-1)}(r)$ appearing in (5.8), taking into account (5.16), we can write

$$H_s^{(0)}(r_0) H_g^{(2n-1)} = H_s^{(0)}(r_0) k H_s^{(2n-2)} + H_s^{(0)}(r_0) \times \int_0^r G_2(r, r_1) V_{21}(r_1) dr_1 \int_0^{r_1} G_1(r_1, r_2) V_{12}(r_2) dr_2 \dots \int_0^{r_{2n-3}} G_1(r_{2n-3}, r_{2n-2}) (V_{12} f_1)_{r_{2n-2}} dr_{2n-2}, \quad (5.17)$$

$$H_s^{(2)}(r_0) H_g^{(2n-3)} = H_s^{(2)}(r_0) k H_s^{(2n-4)} + H_s^{(2)}(r_0) \int_0^r G_2(r, r_1) V_{21}(r_1) dr \times \int_0^{r_1} G_1(r_1, r_2) V_{12}(r_2) dr_2 \dots \int_0^{r_{2n-5}} G_1(r_{2n-5}, r_{2n-4}) (V_{12} f_1)_{r_{2n-4}} dr_{2n-4}, \quad (5.18)$$

$$\dots \dots \dots H_s^{(2n-4)}(r_0) H_g^{(3)} = k H_s^{(2n-4)}(r_0) H_s^{(2)} + H_s^{(2n-4)}(r_0) \int_0^r G_1(r, r_1) (V_{12} f_1)_{r_1} dr_{r_1}, \quad (5.19)$$

$$H_s^{(2n-2)}(r_0) H_g^{(1)} = k H_s^{(2n-2)}(r_0) H_s^{(0)} + H_s^{(2n-2)}(r_0) f_1. \quad (5.20)$$

Quite similar relations can be obtained for the counterterms in (5.8) from the above ones by means of the exchange $r \rightarrow r_0$ in the arguments of $H_s^{(i)}$ and f_1 . In the sum appearing in (5.8), terms and counterterms proportional to k cancel one another; more precisely, the first term cancels the last counterterm, the second term cancels the last but one counterterm, and so on. The sum of the remaining terms can be written as

$$H_s^{(2n-2)}(r_0) f_1 - H_s^{(2n-2)} f_1(r_0) + \left[\sum_{j=0}^{n-3} (H_s^{(2j)}(r_0) H_g^{(2n-2j-3)} - H_s^{(2j)} H_g^{(2n-2j-3)}(r_0)) \right] U_g^{(0)} - f_2, \quad (5.21)$$

where it is understood that the formal replacement $U_g^{(0)} \rightarrow f_2$ has to be made in the integrals expressing any $H_g^{(v)}$. The sum appearing in the above expression is similar to that relative to (5.8) with the substitution $n \rightarrow n-1$. Taking into account (5.14) and (5.15) at any

step we finally obtain

$$\Lambda^{(n)}(r_0, r') = \sum_{j=0}^{n-1} (H_s^{(n-j-1)}(r_0) f_{2j+1}(r') - H_s^{(n-j-1)}(r') f_{2j+1}(r_0)), \quad (5.22)$$

which, by means of (5.6) and (5.7), allows us to get the final expression for u .

6. MAJORIZATION FOR $S^{(n)}$

From (5.10) and (5.11) together with (3.10), (3.24), (3.25), and (4.8) one gets

$$|f_1(r)| < \frac{C_0 C_1 r^{-1}}{|\omega|^5} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g], \quad (6.1)$$

where C_0 denotes a determination of the constant C appearing in (3.10).

Now from (3.10), (3.14), and (4.8) we obtain a majorization for $G_1(r, r')$ which is the same as (I. A6); making use of such majorization together with $|V_{12}| < C|\omega|^{-2}$ in (5.13), we can write

$$|f_2(r)| < \frac{C_0 C_1 C_2 r^{-1}}{|\omega|^8} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g]. \quad (6.2)$$

The majorization procedure can now be extended straightforwardly to (5.14),

$$\left| \frac{f_{2n+1}}{r^{-1} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| W_g]} \right| < \frac{C_0 C_1 (C_1 C_2)^n}{|\omega|^{8n+5}} < \frac{C^{2n+2}}{|\omega|^{8n+5}}, \quad (6.3)$$

where C is the largest constant among C_0, C_1 , and C_2 .

Again taking into account the above cited majorizations for $G_1(r, r')$, V_{12} and making use of (6.3), (4.15), (4.1), (3.10), and (5.7), one gets

$$|S^{(n)}| < \frac{C^{n+2}}{|\omega|^{8n}} [L(|x_g|)]^{l+1} n C \frac{\exp[|\operatorname{Im} \omega| (W_g + W_0)]}{|H_s(r_0)|}. \quad (6.4)$$

From the above inequality and from (5.6) it follows that

$$\left| \sum_{n=m}^{\infty} S^{(n)} \right| < \frac{C^2 \xi^m}{H_s(r_0)} [L(|x_g|)]^{l+1} \exp[|\operatorname{Im} \omega| (W_g + W_0)] \times C \left(\frac{\xi}{(1-\xi)^2} + \frac{m}{1-\xi} \right), \quad (6.5)$$

$$\xi = C/|\omega|^8. \quad (6.6)$$

From the results of Secs. 3 and 4 it follows that⁸

$$H_s(r_0) \approx H_s^{(0)}(r_0) \approx \eta_s^{(0)}(r_0), \quad (6.7)$$

and then from the explicit evaluation of $\eta_s^{(0)}(r_0)$ by means of (I. 3.18),

$$|H_s(r_0)| \approx |\eta_s^{(0)}(r_0)| \approx \frac{C \exp[|\operatorname{Im} \omega| W_0]}{|\omega|^{\bar{r}}}. \quad (6.8)$$

So from (6.4), (6.7), and (6.8) one sees that u near the star surface is proportional to $\exp[|\operatorname{Im} \omega| W_g(r_0)]$ times powers of ω^{-1} .

7. ZEROES OF THE WRONSKIAN

Let us now consider the Wronskian $W(u, u_-)$, whose zeroes give the eigenfrequencies of the star.

From (5.6)–(5.8), recalling the transformation property of the Wronskian for two independent solutions of a second order linear differential equation, we obtain

$$W(u, u_-) = W(U_g^{(0)}, u_-) - \frac{1}{H_s(r_0)} \times \sum_{n=1}^{\infty} \int_0^r \frac{(u_- V_{12})_{r'} \Lambda^{(n)}(r_0, r')}{\exp(\int_{r'}^r B_1(r'') dr'')} dr', \quad (7.1)$$

where B_1 is the coefficient of u' in (I.2.10). The external amplitude u_- is defined by the integral equation (I.5.3) only for $\text{Im}\omega \geq 0$, so that the analytical continuation of u_- to the region $\text{Im}\omega < 0$ is necessary in order to evaluate $W(u, u_-)$ everywhere.

Making use of (I.5.3) and recalling that $U_g^{(0)}$ and $u_g^{(0)}$ are respectively solutions of (2.1) and (I.3.16), we get

$$W(U_g^{(0)}, u_-) = W(u_g^{(0)}, u_-^{(0)}) \left[1 + \frac{\Gamma(\omega)}{\omega} \right], \quad (7.2)$$

$$\Gamma(\omega) = -\omega \int_0^{\infty} \frac{u_g^{(0)} V_{11} u_-}{W(u_g^{(0)}, u_-^{(0)})} dr. \quad (7.3)$$

As shown in paper I, in the region $\text{Im}\omega \geq 0$ we have

$$u_- = u_-^{(0)} + o(u_-^{(0)}), \quad \omega \rightarrow \infty. \quad (7.4)$$

Recalling the definition of $u_g^{(0)}, u_-$ and using a standard relation between Bessel functions of order l we get

$$W(u_g^{(0)}, u_-^{(0)}) = -\omega \phi_g^2 \exp[(\lambda - \nu)/2]. \quad (7.5)$$

Moreover, introducing for them majorizations similar to (3.10) and (3.14) we obtain for $\text{Im}\omega \geq 0$

$$|\Gamma(\omega)| < C, \quad \omega \rightarrow \infty. \quad (7.6)$$

Let us now assume that the above inequality, together with (7.3), also holds for $\text{Im}\omega < 0$.

The proof of the validity of such assumptions rests on the possibility of analytical continuation of u_- and will be the object of another paper. The extension of (7.4) to the half-plane $\text{Im}\omega < 0$ amounts to stating that the asymptotic expression of the analytical continuation is given by the continuation of the asymptotic expression.

We report the results of the asymptotic calculation of the term $n=1$; this is obtained with the help of integration techniques developed in the Appendix, together with the following equality (which derives from standard relations among Bessel functions),

$$\frac{\eta_s^{(0)} \eta_{\sigma, l+1}^{(0)} - \eta_{s, l+1}^{(0)} \eta_{\sigma}^{(0)}}{W(\eta_s^{(0)}, \eta_{\sigma}^{(0)})} = -v_s \frac{\exp[(\nu - \lambda)/2]}{\omega}, \quad (7.7)$$

where

$$\eta_{\sigma, l+1}^{(0)} = \phi_s \left\{ \theta(r - \bar{r}) \exp(-|\text{Im}\omega| W_0) \bar{h}_{l+1}^{(0)}(X) + \theta(\bar{r} - r) [c_s \bar{h}_{l+1}^{(0)}(x_s) + c \bar{h}_{l+1}^{(0)}(x_s)] \right\}. \quad (7.8)$$

We express $\Lambda^{(1)}(r, r')$ by means of (5.22), taking $n=1, j=0$, together with (5.10)–(5.12).

Let us write

$$\Lambda^{(1)}(r, r') = \Lambda_0^{(1)}(r, r') + R_A^{(1)}(r, r'); \quad (7.9)$$

$\Lambda_0^{(1)}$ is the “zero order approximation” for $\Lambda^{(1)}$ in the sense specified in the Appendix, evaluated with the substitutions

$$U_g^{(0)} - U_g^{(0,0)} = u_g^{(0)}, \quad U_{\sigma}^{(0)} - U_{\sigma}^{(0,0)} = u_{\sigma}^{(0)}, \\ H_s^{(0)} - H_s^{(0,0)} = \eta_s^{(0)}, \quad H_{\sigma}^{(0)} - H_{\sigma}^{(0,0)} = \eta_{\sigma}^{(0)}, \quad (7.10)$$

In the numerators of (5.10) and (5.11).

$R_A^{(1)}(r, r')$ is comprehensive both of the higher order iterations describing self-interactions and of remainders to integrals involved in (5.12) together with (7.10) and (7.11).

Similar considerations can be also made for the successive integral $I^{(1)}$ implied in (7.1) in the case $n=1$; again its zero order approximation $I_0^{(1)}$ is obtained by means of the substitution $\Lambda^{(1)}(r, r') - \Lambda_0^{(1)}(r, r')$ together with the substitutions (7.10) in the numerator of $G_1(r, r')$, given by (2.13).

Using (3.10), (3.14), (3.24), (3.25), (4.8), (4.9), and (3.9) together with analogous relations for $U_{\sigma}^{(0,n)}, H_s^{(0,n)}, H_{\sigma}^{(0,n)}$, it is long, but without difficulties and completely in the spirit of the majorization procedures outlined in Sec. 3, to show that the following quantities are negligible for $\omega \rightarrow \infty$ in the expression between brackets in (7.1):

- (i) The integral implying $R_A^{(1)}(r, r')$;
- (ii) The remainder to $I_0^{(1)}$ in the sense of the Appendix;
- (iii) The contributions to $I^{(1)}$ arising from the neglected terms in $G_1(r, r')$, which describe self-interactions;
- (iv) The overall contribution $\sum_{n=2}^{\infty} I^{(n)}$, arising from terms of order $n > 1$;

The calculations lead to

$$I^{(1)} \approx I_0^{(1)} \approx \frac{1}{2\omega} \eta_s^{(0)} \phi_g^2 \left[\bar{j}_l(x_g) \left(\bar{h}_l^{(*)}(x_g) - \frac{l+1}{x_g} \bar{h}_{l+1}^{(*)}(x_g) \right) + \bar{j}_{l+1}(x_g) \left(\bar{h}_{l+1}^{(*)}(x_g) - \frac{l+1}{x_g} \bar{h}_l^{(*)}(x_g) \right) \right] \times \int_0^{w_g(r_0)} \frac{V_{12} V_{21} v_s \exp(\nu - \lambda)}{(1 - v_s^2) W(H_s^{(0)}, H_{\sigma}^{(0)})} dW_g. \quad (7.11)$$

So let us introduce (7.11) together with (4.9) and (6.7) in (7.1) and replace for $\bar{h}_l^{(*)}(x_g)$ and $\bar{j}_l(x_g)$ ($\nu=l, l+1$) their asymptotic expressions for $x_g \rightarrow \infty$.

Then, recalling that $V_{12} V_{21} \sim \omega^{-6}$ and changing sign to ω according to the final remark made in Sec. 1, in the framework of the assumptions we have done, we conclude that the asymptotic eigenfrequencies of the star are given by the equation

$$1 + \frac{\alpha}{i\omega} \Pi \exp[-2i\omega W_g(r_0)] = 0, \quad (7.12)$$

where the real ω -independent constant α is given by

$$\alpha = (-1)^{l+1} \frac{l+1}{2} \left(\frac{\exp[(\nu - \lambda)/2]}{W_\varepsilon^2} \right) \times \int_0^{W_\varepsilon(r_0)} \frac{(\lim_{\omega \rightarrow \infty} V_{12} V_{21} \omega^6) \exp[3(\nu - \lambda)/2]}{\phi_s^2[(1/\nu_s) - 1]} dW_\varepsilon. \quad (7.13)$$

The zeroes of (7.12) are symmetrically distributed with respect to the imaginary axis, and for $\text{Re}\omega > 0$ are asymptotically given by

$$\text{Re}\omega_n \approx \frac{(2n + \frac{1}{2})\pi + \arg\alpha}{2W_\varepsilon(r_0)}, \quad (7.14)$$

$$\text{Im}\omega_n \approx \frac{11 \ln|\text{Re}\omega_n| \text{Re}\omega_n - \ln|\alpha|}{2W_\varepsilon(r_0)}, \quad (7.15)$$

where n is an arbitrary integer such that the rhs of (7.14) is positive. As seen from the above results, the dependence of the ω_n 's on the coupling between the sound and the gravitational waves (contained in α) is weak.

8. FINAL REMARKS

The eigenfrequencies are equally spaced with respect to the real axis of the ω plane and are distributed along a logarithmic curve.

This is also the case for the energy eigenvalues of a particle in a spherically symmetric truncated potential in wave mechanics.⁵

It is easy to see that a similar distribution also occurs in the simpler case of a system⁹ made of two uniform parallel strings of different nature coupled together with transversal uniformly distributed identical springs according to Fig. 1, where A, B , and C are fixed points and string 1 is indefinite towards the right.

The system can be compared with a neutron star radiating gravitational waves; to be definite, strings 1 and 2 can be respectively compared with the physical space (thought of as the medium which propagates the gravitational radiation) and the matter in the star (through which sound waves are propagated). We note that in our case the asymptotic distribution of the eigenfrequencies depends on the equilibrium structure essentially through $W_\varepsilon(r_0)$, which can be interpreted as the optical path of the (uncoupled) gravitational waves throughout the star. With the constant α is associated only a finite "displacement," which is the same for the various eigenfrequencies.

Another observation, which may be relevant for the completeness of eigenmodes, is that the asymptotic zeroes are simple.

APPENDIX

The aim of this appendix is to give a method of successive approximations for large values of $|\omega|$, for integrals which are involved in the iterations for U, H ;

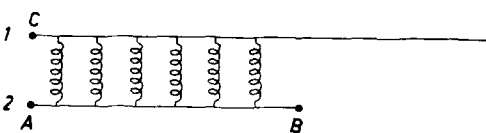


FIG. 1. Coupled springs simulating the interaction of the gravitational field with the neutron star matter.

these belong to the general type

$$I = \int_a^x [A^{(0)} \varphi_l(\omega \Phi_1) \bar{\varphi}_{l'}(\omega \Phi_2) + B^{(0)} \varphi_{l+1}(\omega \Phi_1) \bar{\varphi}_{l'}(\omega \Phi_2) + C^{(0)} \varphi_l(\omega \Phi_1) \bar{\varphi}_{l'+1}(\omega \Phi_2) + D^{(0)} \varphi_{l+1}(\omega \Phi_1) \bar{\varphi}_{l'+1}(\omega \Phi_2)]_x dx', \quad (A1)$$

where $a=0$ or ∞ respectively, for internal and external solutions, $\varphi_{l+j}, \bar{\varphi}_{l'+j_1}$ ($j, j_1=0, 1$) denote the product of spherical Bessel functions of order $l+j, l'+j_1$ times their respective arguments $\omega \Phi_1$ and $\omega \Phi_2$, Φ_1 and Φ_2 being functions of x only; $A^{(0)}, B^{(0)}, C^{(0)}$, and $D^{(0)}$ are functions of x and ω ; we assume that in the limit $\omega \rightarrow \infty$ these are "slowly varying" functions of x , compared with $\varphi_{l+j}, \bar{\varphi}_{l'+j_1}$, which exhibit an exponential behavior of the type $\exp(i\omega \Phi_k)$; it must be understood that φ_l and φ_{l+1} are constructed with Bessel functions of the same kind, namely the coefficients of the linear combination expressing φ_{l+1} in terms of j_{l+1} and n_{l+1} , are the same as those relative to the linear combination expressing φ_l in terms of j_l, n_l ; similarly, $\varphi_{l'}$ and $\varphi_{l'+1}$ are of the same kind (though this may be different from that relative to φ_l, φ_{l+1}). Let us first consider the case $\Phi_1 \neq \Phi_2$, to be distinguished from the case $\Phi_1 = \Phi_2$. For the primitive relative to the integral (A1) we shall tentatively assume a form similar to the integrand

$$P = a \varphi_l \bar{\varphi}_{l'} + b \bar{\varphi}_{l'+1} \varphi_{l'} + c \varphi_l \bar{\varphi}_{l'+1} + d \varphi_{l+1} \bar{\varphi}_{l'+1}, \quad (A2)$$

where a, b, c , and d are to be determined by a method of successive approximations. Owing to a property of Bessel functions, we have

$$\frac{d\varphi_l}{dx} = \omega \frac{d\Phi_1}{dx} \left(-\varphi_{l+1} \frac{l+1}{\omega \Phi_1} \varphi_l \right), \quad (A3)$$

$$\frac{d\varphi_{l+1}}{dx} = \omega \frac{d\Phi_1}{dx} \left(\varphi_l - \frac{l+1}{\omega \Phi_1} \varphi_{l+1} \right),$$

and similar relations for $\bar{\varphi}_{l'}, \bar{\varphi}_{l'+1}$. Then the derivative of P with respect to x can be written as a sum S of terms, originating from the first terms in the rhs's of (A3) (explicitly proportional to ω), plus other terms whose sum we denote by $-T$.

In our problem, in the interval $0 \leq r \leq \bar{r}$, we have the case $l'=l, \Phi_1 = W_\varepsilon, \Phi_2 = W_s$; in such case we choose the zero order approximation $a^{(0)}, b^{(0)}, c^{(0)}$, and $d^{(0)}$ for a, b, c , and d identifying S with the integrand of (A1); in this way one gets

$$a^{(0)} = (\omega F)^{-1} (\Phi_1' B^{(0)} - \Phi_2' C^{(0)})$$

$$b^{(0)} = -(\omega F)^{-1} (\Phi_1' A^{(0)} + \Phi_2' D^{(0)}) \quad (A4)$$

$$c^{(0)} = (\omega F)^{-1} (\Phi_1' D^{(0)} + \Phi_2' A^{(0)})$$

$$d^{(0)} = -(\omega F)^{-1} (\Phi_1' C^{(0)} - \Phi_2' B^{(0)}),$$

$$F = (\Phi_2')^2 - (\Phi_1')^2, \quad \Phi_1' = \frac{d\Phi_1}{dx}, \quad \Phi_2' = \frac{d\Phi_2}{dx}, \quad (A5)$$

$$I = [a^{(0)} \varphi_l \bar{\varphi}_{l'} + b^{(0)} \varphi_{l+1} \bar{\varphi}_{l'} + c^{(0)} \varphi_l \bar{\varphi}_{l'+1} + d^{(0)} \varphi_{l+1} \bar{\varphi}_{l'+1}]_a^x + \int_a^x T dr'. \quad (A6)$$

Now the integral in the rhs of the above equality has a structure which is similar to that of the original integral (A1); however its coefficients, compared with

$A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$, exhibit an explicit factor $1/\omega$ as seen from (A4); we can therefore apply a similar procedure to such an integral, and so on. In this way one obtains a method of successive approximations for I when $|\omega|$ is large. The m th approximation is written as:

$$I = \sum_{n=0}^m [a^{(n)} \varphi_1 \bar{\varphi}_1 + b^{(n)} \varphi_{l+1} \bar{\varphi}_1 + c^{(n)} \varphi_1 \bar{\varphi}_{l+1} + d^{(n)} \varphi_{l+1} \bar{\varphi}_{l+1}]_a^x + \int_a^x [A^{(m+1)} \varphi_1 \bar{\varphi}_1 + B^{(m+1)} \varphi_{l+1} \bar{\varphi}_1 + C^{(m+1)} \varphi_1 \bar{\varphi}_{l+1} + D^{(m+1)} \varphi_{l+1} \bar{\varphi}_{l+1}] dx', \quad (\text{A7})$$

$$a^{(n+1)} = (\omega F)^{-1} (\Phi_1' B^{(n+1)} - \Phi_2' C^{(n+1)}),$$

$$b^{(n+1)} = -(\omega F)^{-1} (\Phi_1' A^{(n+1)} + \Phi_2' D^{(n+1)}), \quad (\text{A8})$$

$$c^{(n+1)} = (\omega F)^{-1} (\Phi_1' D^{(n+1)} + \Phi_2' A^{(n+1)}),$$

$$d^{(n+1)} = -(\omega F)^{-1} (\Phi_1' C^{(n+1)} - \Phi_2' B^{(n+1)}),$$

$$A^{(n+1)} = -\left(\frac{da^{(n)}}{dx} + T_+ a^{(n)}\right), \quad C^{(n+1)} = -\left(\frac{dc^{(n)}}{dx} + T_- c^{(n)}\right), \quad (\text{A9})$$

$$B^{(n+1)} = -\left(\frac{db^{(n)}}{dx} - T_- b^{(n)}\right), \quad D^{(n+1)} = -\left(\frac{dd^{(n)}}{dx} - T_+ d^{(n)}\right),$$

$$T_{\pm} = \frac{l+1}{\Phi_1} \Phi_1' \pm \frac{l+1}{\Phi_2} \Phi_2', \quad (\text{A10})$$

where the integral in the rhs of (A7) is the remainder of order m of the development of I into successive approximations; an overall factor $1/\omega^{m+1}$ can be extracted from it.

The question is left whether the integrals of type (A1) are convergent in the case of interest. To this aim some observations and assumptions, bearing on the structure of Φ_1 , Φ_2 , $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$, are necessary. We note that Φ_1' , Φ_2' , given by (A5) are respectively equal to $\exp(\lambda - \nu)/2$, $[\exp(\lambda - \nu)/2]/v_s$, where v_s is the velocity of sound; Φ_1' , Φ_2' , for a neutron star, are finite, different from zero and from one another, so that F , given by (A5) satisfies the inequality $|1/F| < C$.

Now let us make the following assumptions:

(1) The equation of state is such that Φ_1' , Φ_2' , λ , ν are analytical in r for $r=0$.

(2) $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are majorized by a constant C , for $0 \leq r \leq \bar{r}$, together with their derivatives with respect to r up to a certain order q .

(3) $A^{(0)}$ and $D^{(0)}$ are even functions of r for $r \rightarrow 0$, whereas $B^{(0)}$ and $C^{(0)}$ are odd.¹⁰

From (1) we conclude that T_{\pm} , as given by (A10), in the case under examination ($l'=l$), is an odd function of r and vanishes as r for $r \rightarrow 0$.

From (A8) and (A9), and from the above assumptions and results one proves by induction that $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, $A^{(n+1)}$, $B^{(n+1)}$, $C^{(n+1)}$, and $D^{(n+1)}$ are majorized by a constant C for $0 \leq r \leq \bar{r}$, $n \leq q$ and that $b^{(n)}$, $c^{(n)}$, $A^{(n+1)}$, and $D^{(n+1)}$ are even functions of r for $r \rightarrow 0$, whereas, $a^{(n)}$, $d^{(n)}$, $B^{(n+1)}$, and $C^{(n+1)}$ are odd.

Let us further consider the case $\bar{l}=l'$, $\Phi_1 = W_{\epsilon}$, $\Phi_2 = x = W_s - W_s(r_0)$, $\bar{r} \leq r \leq r_0$, which is also involved in our problem; in this case the Bessel functions with index \bar{l} , $\bar{l}+1$ may diverge respectively as $x^{-\bar{l}}$, $x^{-(\bar{l}+1)}$ on the star surface. However, these are always multiplied by coefficients containing a factor x^{α} with $\alpha = \bar{l}+1$.

With reference to (A1) let us write such coefficients in the form:

$$A^{(0)} = f_1^{(0)} x^{\alpha}, \quad B^{(0)} = f_2^{(0)} x^{\alpha},$$

$$C^{(0)} = f_3^{(0)} x^{\alpha}, \quad D^{(0)} = f_4^{(0)} x^{\alpha}.$$

With reference to the primitive (A2) we set

$$a = \bar{a} x^{\alpha}, \quad b = \bar{b} x^{\alpha}, \quad c = \bar{c} x^{\alpha}, \quad d = \bar{d} x^{\alpha}. \quad (\text{A11})$$

In order to determine the lowest order approximation $\bar{a}^{(0)}$, $\bar{b}^{(0)}$, $\bar{c}^{(0)}$, and $\bar{d}^{(0)}$, we formally write \bar{a} , \bar{b} , \bar{c} , and \bar{d} in the form

$$\bar{a} = \sum_n \bar{a}^{(n)}, \quad \bar{b} = \sum_n \bar{b}^{(n)}, \quad (\text{A12})$$

$$\bar{c} = \sum_n \bar{c}^{(n)}, \quad \bar{d} = \sum_n \bar{d}^{(n)}.$$

Let us further replace (A11) and (A12) into the derivative with respect to x of (A2), and equate the coefficients of φ_{l+j} , $\varphi_{\bar{l}+j_1}$ ($j, j_1 = 0, 1$) relative to the largest power of ω in such a derivative with the analogous coefficients in the integrand of (A1).

In this way we obtain:

$$\bar{a}^{(0)} = \frac{v_s f_2^{(0)} - f_3^{(0)}}{\omega F}, \quad \bar{b}^{(0)} = -\frac{f_4^{(0)} + v_s f_1^{(0)}}{\omega F}, \quad (\text{A13})$$

$$\bar{c}^{(0)} = \frac{f_1^{(0)} + v_s f_4^{(0)}}{\omega F}, \quad \bar{d}^{(0)} = \frac{f_2^{(0)} - v_s f_3^{(0)}}{\omega F}.$$

Then the integral I can be written as

$$(\bar{a}^{(0)} \varphi_1 \bar{\varphi}_1 + \bar{b}^{(0)} \varphi_{l+1} \bar{\varphi}_1 + \bar{c}^{(0)} \varphi_1 \bar{\varphi}_{l+1} + \bar{d}^{(0)} \varphi_{l+1} \bar{\varphi}_{l+1}) x^{\alpha} + \int_x^x [x^{\alpha} (f_1^{(1)} \varphi_1 \bar{\varphi}_1 + f_2^{(1)} \varphi_{l+1} \bar{\varphi}_1 + f_3^{(1)} \varphi_1 \bar{\varphi}_{l+1} + f_4^{(1)} \varphi_{l+1} \bar{\varphi}_{l+1})]_x' dx', \quad (\text{A14})$$

where:

$$f_1^{(1)} = -\frac{1}{\omega} \left[\frac{v_s f_2^{(0)} - f_3^{(0)}}{F} \left(\frac{l+1}{W_{\epsilon}} v_s + 2 \frac{\bar{l}+1}{x} \right) + \frac{d}{dx} \left(\frac{v_s f_2^{(0)} - f_3^{(0)}}{F} \right) \right],$$

$$f_2^{(1)} = \frac{1}{\omega} \left[\frac{f_4^{(0)} + v_s f_1^{(0)}}{F} \left(2 \frac{\bar{l}+1}{x} - \frac{l+1}{W_{\epsilon}} v_s \right) + \frac{d}{dx} \left(\frac{f_4^{(0)} + v_s f_1^{(0)}}{F} \right) \right],$$

$$f_3^{(1)} = -\frac{1}{\omega} \left[\frac{l+1}{W_{\epsilon}} v_s \frac{f_1^{(0)} + v_s f_4^{(0)}}{F} + \frac{d}{dx} \left(\frac{f_1^{(0)} + v_s f_4^{(0)}}{F} \right) \right],$$

$$f_4^{(1)} = -\frac{1}{\omega} \left[\frac{l+1}{W_{\epsilon}} v_s \frac{v_s f_3^{(0)} - f_2^{(0)}}{F} + \frac{d}{dx} \left(\frac{v_s f_3^{(0)} - f_2^{(0)}}{F} \right) \right]. \quad (\text{A15})$$

The integral in the rhs of (A14) belongs to the same type as (A1); however, its coefficients, compared to

those of (A1), contain an additional factor $1/\omega$; we can thus set up a method of successive approximations for I for large values of $|\omega|$ by treating such an integral in a way similar to the previous one, and so on. The m th approximation reads

$$I = \sum_{n=0}^m [x^\alpha (\bar{a}^{(n)} \varphi_i \bar{\varphi}_i + \bar{b}^{(n)} \varphi_{i+1} \bar{\varphi}_i + \bar{c}^{(n)} \varphi_i \bar{\varphi}_{i+1} + \bar{d}^{(n)} \varphi_{i+1} \bar{\varphi}_{i+1})]_x^\alpha + \int_x^\alpha [x^\alpha (f_1^{(m+1)} \varphi_i \bar{\varphi}_i + f_2^{(m+1)} \varphi_{i+1} \bar{\varphi}_i + f_3^{(m+1)} \varphi_i \bar{\varphi}_{i+1} + f_4^{(m+1)} \varphi_{i+1} \bar{\varphi}_{i+1})]_{x'} dx', \quad (\text{A16})$$

where $f_k^{(m+1)}$ are related to $f_j^{(m)}$ ($k, j = 1, 2, 3, 4$) by the same relationships as those between $f_k^{(1)}$ and $f_j^{(0)}$, namely (A15); $\bar{a}^{(n)}$, $\bar{b}^{(n)}$, $\bar{c}^{(n)}$, and $\bar{d}^{(n)}$ are formally obtained from (A13) with the substitution of the index (0) with the index (n). Also in this case it must be verified that the successive approximations and their remainders are finite in the range of interest $\bar{r} \leq r \leq r_0$.

To this aim let us assume that:

- (4) $f_k^{(0)}$ are majorized by a constant C together with their derivatives up to a certain order q .
- (5) $f_1^{(0)}$ and $f_2^{(0)}$ behave like even functions of x in the limit $x \rightarrow 0$, whereas $f_3^{(0)}$ and $f_4^{(0)}$ behave like odd functions in the same limit.
- (6) $f_k^{(0)}$ are analytical in r in a certain neighborhood of $r = r_0$.¹¹

It easily follows by induction from (A13) and (A15) that $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, and $f_k^{(n+1)}$ are majorized by a constant C for $n \leq q$; in addition $f_1^{(n+1)}$, $f_2^{(n+1)}$, $c^{(n)}$, and $d^{(n)}$ behave like even function of x for $x \rightarrow 0$, whereas $f_3^{(n+1)}$, $f_4^{(n+1)}$, $a^{(n)}$, and $b^{(n)}$ behave like odd functions in the same limit for $n \leq q$.

Let us finally give a similar approach for integrals of type (A1) with $\Phi_1 = \Phi_2$; for the purpose of the present paper it will be enough to consider the case $l = l'$. Since the coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are arbitrary, we assume the variable x to coincide with $\Phi_1 = \Phi_2$.

First of all, integrating the last term of (A1) by parts we obtain, by means of (A3),

$$\int_x^\alpha D^{(0)} \varphi_{i+1} \bar{\varphi}_{i+1} dx' = \frac{1}{\omega} \int_x^\alpha \frac{dD^{(0)}}{dx} \varphi_i \bar{\varphi}_{i+1} dx' + \int_x^\alpha D^{(0)} \varphi_i \bar{\varphi}_i dx' - \frac{1}{\omega} D^{(0)} \varphi_i \bar{\varphi}_{i+1}, \quad (\text{A17})$$

moreover, recalling that, owing to a property of Bessel functions, the expression $\varphi_i \bar{\varphi}_{i+1} - \bar{\varphi}_i \varphi_{i+1}$ is a constant, again with the help of (A3), one obtains by further partial integrations

$$\begin{aligned} & \int_x^\alpha (f_1 \varphi_{i+1} \bar{\varphi}_i + f_2 \varphi_i \bar{\varphi}_{i+1}) dx' \\ &= \frac{1}{\omega} \int_x^\alpha \left[\frac{l+1}{x} (f_1 + f_2) + \frac{1}{2} \frac{d}{dx} (f_1 + f_2) \right]_{x'} \varphi_i \bar{\varphi}_i dx' \\ &+ \frac{1}{2} (\varphi_{i+1} \bar{\varphi}_i - \varphi_i \bar{\varphi}_{i+1}) \int_0^x (f_1 - f_2) dx' - \frac{1}{2\omega} (f_1 + f_2) \varphi_i \bar{\varphi}_i, \end{aligned} \quad (\text{A18})$$

where f_1 and f_2 are slowly varying functions.

Using up the above relations for the primitive P of (A1) we get

$$P = \int_x^\alpha f^{(0)} \varphi_i \bar{\varphi}_i dx' + \frac{1}{2} (\varphi_{i+1} \bar{\varphi}_i - \varphi_i \bar{\varphi}_{i+1}) \times \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right) dx' - \frac{1}{\omega} D^{(0)} \varphi_i \bar{\varphi}_{i+1} - \frac{1}{2\omega} \left(B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right) \varphi_i \bar{\varphi}_i, \quad (\text{A19})$$

$$f^{(0)} = A^{(0)} + D^{(0)} + \left[\frac{l+1}{\omega x} + \frac{1}{2\omega} \frac{d}{dx} \right] \times \left(B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right). \quad (\text{A20})$$

Now using (A3) one can verify the equality (by derivation of both sides)

$$\begin{aligned} & \int_x^\alpha f_i^{(0)} \varphi_i \bar{\varphi}_i dx' \\ &= \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \\ &+ \frac{1}{2} \int_0^x f^{(0)} dx' (\varphi_i \varphi_i + \varphi_{i+1} \varphi_{i+1}) - \frac{1}{4\omega} \int_x^\alpha \left[\frac{d}{dx} \left(f^{(0)} - \frac{2(l+1)}{x'} \int_0^x f^{(0)} dx'' \right) (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \right]_{x'} dx'. \end{aligned} \quad (\text{A21})$$

Then from (A19) and the above equality, one obtains

$$I = [a^{(0)} \varphi_i \bar{\varphi}_i + b^{(0)} \varphi_{i+1} \bar{\varphi}_i + c^{(0)} \varphi_i \bar{\varphi}_{i+1} + d^{(0)} \varphi_{i+1} \bar{\varphi}_{i+1}]_a^\alpha - \frac{1}{4\omega} \int_a^\alpha \left[\frac{d}{dx} \left(f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx'' \right) (\varphi_{i+1} \bar{\varphi}_i + \varphi_i \bar{\varphi}_{i+1}) \right]_{x'} dx', \quad (\text{A22})$$

$$a^{(0)} = \frac{1}{2} \int_0^x f^{(0)} dx' - \frac{1}{2\omega} \left[B^{(0)} + C^{(0)} + \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right],$$

$$b^{(0)} = \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] + \frac{1}{2} \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right)_{x'} dx', \quad (\text{A23})$$

$$c^{(0)} = \frac{1}{4\omega} \left[f^{(0)} - \frac{2(l+1)}{x} \int_0^x f^{(0)} dx' \right] - \frac{1}{2} \int_0^x \left(B^{(0)} - C^{(0)} - \frac{1}{\omega} \frac{dD^{(0)}}{dx} \right)_{x'} dx' - \frac{1}{\omega} D^{(0)},$$

$$d^{(0)} = \frac{1}{2} \int_0^x f^{(0)} dx'.$$

The integral in the rhs of (A22) belongs to the original type (A1); however its coefficients exhibit (at least) a factor $1/\omega$ in comparison with the original coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$.

A similar approach can be applied to this integral, and so on, for the successive approximations. The m th approximation is formally written as (A7) in which

$$A^{(n+1)} = D^{(n+1)} = 0,$$

$$B^{(n+1)} = C^{(n+1)} = -\frac{1}{4\omega} \frac{d}{dx} \left[f^{(n)} - \frac{2(l+1)}{x} \int_0^x f^{(n)} dx' \right], \quad (\text{A24})$$

and $a^{(n+1)}$, $b^{(n+1)}$, $c^{(n+1)}$, and $d^{(n+1)}$ are related to $f^{(n+1)}$ and $B^{(n+1)}$ by the same relationships (A23) which connect $a^{(0)}$, $b^{(0)}$, $c^{(0)}$, and $d^{(0)}$ to $f^{(0)}$, $B^{(0)}$, where formally one sets $C^{(0)} = B^{(0)}$, $D^{(0)} = 0$.

Once again it must be verified that the successive approximations are convergent for $x \rightarrow 0$ in the cases of interest. To this aim we make the following assumptions analogous to (4), (5), and (6).

(7) $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are majorized by a constant C together with their derivatives up to a certain order q , respectively, in the intervals $0 \leq x \leq x(\bar{r})$ when $x = W_g$ or W_s and $0 \geq x \geq W_s(\bar{r}) - W_s(r_0)$ when $x = W_s - W_s(r_0)$.

(8) $A^{(0)}$ and $D^{(0)}$ behave as even functions for $x \rightarrow 0$, whereas $B^{(0)}$ and $C^{(0)}$ behave as odd functions in the same limit.

(9) The coefficients $A^{(0)}$, $B^{(0)}$, $C^{(0)}$, and $D^{(0)}$ are analytical in a neighborhood of $r=0$, or $r=r_0$ according to whether the first or the second interval is considered.¹¹

Then one easily proves by induction that $f^{(n)}$, $a^{(n)}$, $b^{(n)}$, $c^{(n)}$, $d^{(n)}$, and $B^{(n+1)} = C^{(n+1)}$ for $n \leq q$ are majorized by a constant C in the intervals considered in (6),

according to the specifications made there; in addition $b^{(n)}$, $c^{(n)}$, and $f^{(n)}$ have an even character for $x \rightarrow 0$, where $a^{(n)}$, $d^{(n)}$, and $B^{(n+1)} = C^{(n+1)}$ have an odd character in the same limit.

¹P. Cazzola, L. Lucaroni, and R. Semenzato, *J. Math. Phys.* **19**, 237 (1978).

²For the definition of W_s , W_g see (I.3.19) [paper I above, Eq. (3.19)].

³P. Cazzola and L. Lucaroni, *Phys. Rev. D* **6**, 950 (1972).

⁴R. G. Newton, *J. Math. Phys.* **1**, 319 (1960).

⁵T. Regge, *Nuovo Cimento* **9**, 295 (1958).

⁶Here and in the following C or C_1, C_2, \dots denote positive ω -independent constants.

⁷One easily verifies that the normalization for u defined in (3) in the limit $r \rightarrow 0$ coincides with the one given by (5.1) and (5.3).

⁸Equation (6.7) holds with the exception of those values of ω in the real axis for which $\eta_s^{(0)}(r_0)$ vanishes; but these never coincide with the eigenfrequencies in which we are interested.

⁹L. Battiston, P. Cazzola, and L. Lucaroni, *Nuovo Cimento B* **3**, 295 (1971).

¹⁰We note that 2) can be verified by inspection, whereas Φ'_1 , Φ'_2 , λ , ν are even functions of r in a neighborhood of $r=0$ as a consequence of the equilibrium equations. 3) follows from the above statement and from the definite parity character of the coefficients of the coupled equations (I.2.10) and (I.2.23).

¹¹For the integrals involved in our problem 4), 7) can be verified by inspection. As regards 5), 6), 8), 9) it is evident that, even if they do not hold, the above formulas are valid up to a certain order of approximation such that, at any step, the coefficients of the cited byproducts in the remainders are finite. Since in the calculation of the integrals involved in Secs. 5 and 7 it is sufficient to consider the lowest order approximations, we can see by inspection that the above conditions are satisfied. The remainders are then majorized according to standard procedures developed in paper I or in Sec. 3, and are shown to be negligible.

Diffraction by two parallel slits in a plane

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The diffraction of scalar waves by two parallel slits in a plane screen is examined by a method which uses orthogonal functions and Fourier transformations. A solution is obtained in the case of a perfectly soft screen. Numerical results of the plane wave transmission coefficients for normal incidence are given for $k = 0.2 \sim 4.0$ and $D = 3 \sim 10$, where k is the wavenumber and D is the distance between slits.

1. INTRODUCTION

The present paper deals with the diffraction of scalar waves by two parallel slits in a plane screen. In contrast to the case of the diffraction by a single slit, there have been relatively few investigations on this problem. This is because of the theoretical difficulties due to interaction between slits. So far as we are aware, no exact solution is known. As approximate methods, there are the Kirchhoff-type approximation, the Keller geometrical theory of diffraction^{1,2} and the method of Weber-Schafheitlin integrals,³ which are invalid for small values of the wavenumber and of the distance between slits. Sachdeva and Hurd⁴ obtain a solution which are valid for small values of these parameters, but some of their numerical results are doubtful.⁵

We examine this problem by a method which is based on the use of Fourier transformations of the functions with the bounded support and the expansions by an orthogonal set of functions. This method is efficient for small k and D and has been successfully applied to the problem of the diffraction by a slit.⁶

2. THEORY

Suppose the perfectly soft screen contains two parallel slits of the width $2a$ and choose a rectangular coordinate system so that the screen coincides with the plane $z = 0$ and the center lines of the slits are given by $x = a + 1$ and $x = a - 1$ respectively (see Fig. 1). Let the primary field ϕ_0 which has no y variation be incident from the left ($z < 0$), then the total field ψ is expressed as

$$\psi(x, z) = \begin{cases} \phi_0(x, z) - \phi_0(x, -z) + \phi(x, -z) & (z < 0), \\ \phi(x, z) & (z > 0), \end{cases} \quad (1)$$

where ϕ , to be defined for $z \geq 0$ only, is given by a solution of the following boundary value problem⁷:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \right) \phi = 0 \quad (z > 0), \quad (2)$$

$$\phi = 0 \quad (z = 0, |x| < a, |x| > a + 2), \quad (3)$$

$$\frac{\partial \phi}{\partial z} = \frac{\partial \phi_0}{\partial z} \equiv f(x) \quad (z = 0, a < |x| < a + 2), \quad (4)$$

where k is the wavenumber. Since we discuss a steady-state problem, the time factor $\exp(-i\omega t)$ is omitted throughout. By introducing new variables

$$x_1 = x - a - 1, \quad x_2 = x + a + 1 \quad (5)$$

and new functions

$$f(x) = \begin{cases} f_1(x_1) & (|x_1| < 1), \\ f_2(x_2) & (|x_2| < 1), \end{cases} \quad (6)$$

Eq. (4) is written

$$\frac{\partial \phi}{\partial z} = \begin{cases} f_1(x_1) & (z = 0, |x_1| < 1), \\ f_2(x_2) & (z = 0, |x_2| < 1). \end{cases} \quad (7)$$

The wave equation (2) is separable, and we can assume the following expression as a solution:

$$\phi(x, z) = \sum_{n=0}^{\infty} A_n \int_{-\infty}^{\infty} U_n(s) \exp(isx_1) \exp[-(s^2 - k^2)^{1/2} z] ds + \sum_{n=0}^{\infty} B_n \int_{-\infty}^{\infty} U_n(s) \exp(isx_2) \exp[-(s^2 - k^2)^{1/2} z] ds, \quad (8)$$

where A_n , B_n , and $U_n(s)$ are determined from the boundary conditions. Substituting this solution into Eqs. (3) and (7), we have

$$\begin{aligned} \sum_{n=0}^{\infty} A_n \int_{-\infty}^{\infty} U_n(s) \exp(isx_1) ds \\ + \sum_{n=0}^{\infty} B_n \int_{-\infty}^{\infty} U_n(s) \exp(isx_2) ds = 0 \end{aligned} \quad (9)$$

$(|x| < a, |x| > a + 2)$

and

$$\sum_{n=0}^{\infty} A_n \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_n(s) \exp(isx_1) ds$$

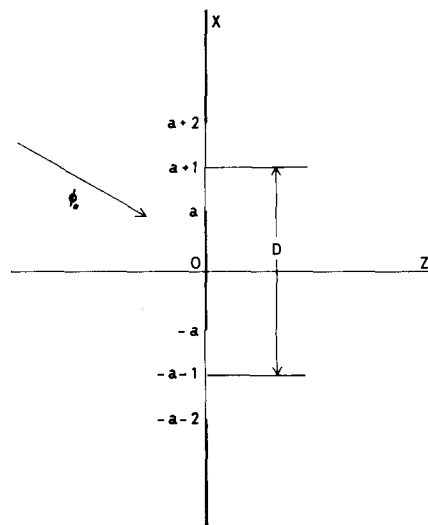


FIG. 1. Configuration of two slits.

$$\begin{aligned}
& + \sum_{n=0}^{\infty} B_n \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_n(s) \exp(isx_2) ds \\
& = \begin{cases} -f_1(x_1) & (|x_1| < 1), \\ -f_2(x_2) & (|x_2| < 1), \end{cases} \quad (10)
\end{aligned}$$

respectively.

Noting that the integrals in Eq. (9) have a form of the Fourier transform, we introduce a complete orthonormal set of functions $\{u_n(x)\}$ ($|x| < 1$, $n = 0, 1, 2, \dots$) which belongs to the weight function $w(x)$ and define a sequence of functions $v_n(x)$ as

$$v_n(x) = \begin{cases} 0 & (|x| > 1), \\ w(x)u_n(x) & (|x| < 1). \end{cases} \quad (11)$$

If we assume that the functions $U_n(s)$ are the Fourier transforms of $v_n(x)$, that is,

$$\begin{aligned}
U_n(s) &= \int_{-\infty}^{\infty} v_n(x) \exp(-isx) dx \\
&= \int_{-1}^1 w(x)u_n(x) \exp(-isx) dx, \quad (12)
\end{aligned}$$

then the inversion formula

$$\int_{-\infty}^{\infty} U_n(s) \exp(isx) ds = 2\pi v_n(x) \quad (13)$$

and Eq. (11) show that one of the boundary conditions (9) is automatically satisfied.

Another boundary condition (10) is written by the use of Eq. (5):

$$\begin{aligned}
& \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_n(s) \exp(isx_1) \\
& \quad \times [A_n + B_n \exp(isD)] ds \\
& = -f_1(x_1) \quad (|x_1| < 1), \quad (14)
\end{aligned}$$

$$\begin{aligned}
& \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_n(s) \exp(isx_2) \\
& \quad \times [A_n \exp(-isD) + B_n] ds \\
& = -f_2(x_2) \quad (|x_2| < 1), \quad (15)
\end{aligned}$$

where $D = 2(a + 1)$. We expand the functions $\exp(isx_1)$ and $f(x_1)$ in Eq. (14) in terms of $u_n(x_1)$, obtaining

$$\exp(isx_1) = \sum_{m=0}^{\infty} E_m^{(1)}(s) u_m(x_1) \quad (16)$$

with

$$E_m^{(1)}(s) = \int_{-1}^1 w(x)u_m(x) \exp(isx) dx = U_m(-s) \quad (17)$$

and

$$-f_1(x_1) = \sum_{m=0}^{\infty} F_m^{(1)} u_m(x_1) \quad (18)$$

with

$$F_m^{(1)} = - \int_{-1}^1 w(x)u_m(x) f_1(x) dx, \quad (19)$$

respectively. Substituting these results into Eq. (14) and changing the order of summation and integration, we have an infinite set of linear equations

$$\sum_{n=0}^{\infty} (P_{mn} A_n + Q_{mn} B_n) = F_m^{(1)} \quad (m = 0, 1, 2, \dots), \quad (20)$$

where

$$\begin{aligned}
P_{mn} &= \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_m(-s) U_n(s) ds \\
&= \int_0^{\infty} (s^2 - k^2)^{1/2} [U_m(s) U_n(-s) + U_m(-s) U_n(s)] ds = P_{nm}
\end{aligned} \quad (21)$$

and

$$Q_{mn} = \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_m(-s) U_n(s) \exp(isD) ds. \quad (22)$$

Similarly, we have from Eq. (15)

$$\sum_{n=0}^{\infty} (R_{mn} A_n + P_{mn} B_n) = F_m^{(2)} \quad (m = 0, 1, 2, \dots), \quad (23)$$

where

$$R_{mn} = \int_{-\infty}^{\infty} (s^2 - k^2)^{1/2} U_m(-s) U_n(s) \exp(-isD) ds = Q_{nm} \quad (24)$$

and

$$F_m^{(2)} = - \int_{-1}^1 w(x)u_m(x) f_2(x) dx. \quad (25)$$

By solving Eqs. (20) and (23), the coefficients A_n and B_n are determined so that another boundary condition (10) is satisfied and the solution for the problem is formally obtained.

When the distance between the slits is sufficiently large, that is, $D \rightarrow \infty$, we have by the Riemann–Lebesgue theorem

$$Q_{mn} = R_{mn} = 0.$$

Then Eqs. (20) and (23) reduce to

$$\sum_{n=0}^n P_{mn} A_n = F_m^{(1)} \quad (m = 0, 1, 2, \dots) \quad (26)$$

and

$$\sum_{n=0}^{\infty} P_{mn} B_n = F_m^{(2)} \quad (m = 0, 1, 2, \dots), \quad (27)$$

respectively, which show that the unknowns A_n and B_n are determined independently and hence the solution is expressed as the algebraic sum of the solutions for the individual slits.⁴

3. CALCULATION OF P_{mn} AND Q_{mn}

From Eqs. (8), (11), and (13) we have for the aperture field

$$\begin{aligned}
\phi(x, 0) &= 2\pi \sum_{n=0}^{\infty} [A_n w(x_1) u_n(x_1) + B_n w(x_2) u_n(x_2)] \\
& \quad (|x_1| < 1, |x_2| < 1).
\end{aligned}$$

For numerical calculation, it is convenient to choose the functions $w(x)$ and $u_n(x)$ so that the above series converges rapidly. Consulting the results for a slit, we take the following functions:

$$u_n(x) = [\Gamma(n+2)/\sqrt{2} \Gamma(n+\frac{3}{2})] P_n^{(1/2, 1/2)}(x) \quad (n = 0, 1, 2, \dots), \quad (28)$$

$$w(x) = (1 - x^2)^{1/2}, \quad (29)$$

where $P_n^{(1/2, 1/2)}(x)$ are the Jacobi polynomials defined by

$$P_n^{(1/2, 1/2)}(x) = \frac{(-1)^n (1 - x^2)^{-1/2}}{2^n \Gamma(n+1)} \frac{d^n}{dx^n} (1 - x^2)^{n+1/2}. \quad (30)$$

Then Eqs. (12), (21), and (22) become

$$U_n(s) = (2\pi)^{1/2}(-i)^n(n+1)J_{n+1}(s)/s, \quad (31)$$

$$P_{mn} = C_{mn} \int_0^\infty (s^2 - k^2)^{1/2} [J_{m+1}(s)J_{n+1}(s)/s^2] ds \quad (32)$$

and

$$Q_{mn} = C_{mn} \int_0^\infty (s^2 - k^2)^{1/2} \cos Ds [J_{m+1}(s)J_{n+1}(s)/s^2] ds \\ + D_{mn} \int_0^\infty (s^2 - k^2)^{1/2} \sin Ds [J_{m+1}(s)J_{n+1}(s)/s^2] ds, \quad (33)$$

respectively, where

$$C_{mn} = 2\pi i^{m+n} [(-1)^m + (-1)^n] (m+1)(n+1), \quad (34)$$

$$D_{mn} = 2\pi i^{m+n+1} [(-1)^n - (-1)^m] (m+1)(n+1). \quad (35)$$

Note that C_{mn} are real and equal to zero if $m+n$ are odd and D_{mn} are real and equal to zero if $m+n$ are even. The integrals of Eqs. (32) and (33) are convergent and we have (see Appendix)

$$P_{mn} = \frac{1}{2}\pi^{3/2}(-1)^\lambda [(-1)^m + (-1)^n] (m+1)(n+1) \\ \times \left[\sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\mu+\lambda} P_1(\mu, \nu) + \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} P_2(\mu, \nu) \right. \\ \left. - i \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} P_3(\mu, \nu) \right] (m+n=2\lambda, \lambda=0, 1, 2, \dots), \quad (36)$$

$$P_{mn} = 0 \quad (m+n=2\lambda+1, \lambda=0, 1, 2, \dots), \quad (37)$$

and

$$Q_{mn} = \frac{1}{2}\pi^2(-1)^\lambda [(-1)^m + (-1)^n] (m+1)(n+1) \\ \times \left[\sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\mu+\lambda} Q_1(\mu, \nu) + \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} Q_2(\mu, \nu) \right. \\ \left. - i \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} Q_3(\mu, \nu) \right] (m+n=2\lambda, \lambda=0, 1, 2, \dots), \quad (38)$$

$$Q_{mn} = \frac{1}{2}\pi^2(-1)^\lambda [(-1)^m - (-1)^n] (m+1)(n+1) \\ \times \left[\sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\mu+\lambda+1} Q_4(\mu, \nu) + \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} Q_5(\mu, \nu) \right. \\ \left. - i \sum_{\mu=0}^{\infty} \sum_{\nu=0}^{\infty} Q_6(\mu, \nu) \right] (m+n=2\lambda+1, \lambda=0, 1, 2, \dots), \quad (39)$$

where

$$P_1(\mu, \nu) = G_1(\mu, \nu) \frac{(-1)^{\mu+\nu}\Gamma(\mu-\nu+\lambda+1)}{\Gamma(\nu-\mu-\lambda+n+1)\Gamma(-\nu+3/2)} \left(\frac{k}{2}\right)^{2\nu},$$

$$P_2(\mu, \nu) = G_1(\mu, \nu) \\ \times \frac{(-1)^\lambda \psi_1(\mu, \nu)}{\Gamma(\mu+\nu+\lambda+2)\Gamma(\nu+n+2)\Gamma(-\mu-\nu-\lambda+1/2)} \\ \times \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+1)}$$

$$P_3(\mu, \nu) = G_1(\mu, \nu) \frac{(-1)^{\mu+\nu}\Gamma(\mu+\nu+\lambda+1/2)}{\Gamma(\mu+\nu+\lambda+2)\Gamma(\nu+n+2)} \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+1)},$$

$$Q_1(\mu, \nu) = G_2(\mu, \nu) \frac{(-1)^{\mu+\nu}\Gamma(\mu-\nu+\lambda+1)}{\Gamma(\nu-\mu-\lambda-1/2)\Gamma(-\nu+3/2)} \\ \times \left(\frac{k}{2}\right)^{2\nu} D^{2(\nu-\mu-\lambda-1)},$$

$$Q_2(\mu, \nu) = G_2(\mu, \nu) \\ \times \frac{(-1)^\lambda \psi_2(\mu, \nu)}{\Gamma(\mu+\nu+\lambda+2)\Gamma(\nu+1/2)\Gamma(-\mu-\nu-\lambda+1/2)}$$

$$\times \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+1)} D^{2\nu},$$

$$Q_3(\mu, \nu) = G_2(\mu, \nu) \\ \times \frac{(-1)^{\mu+\nu}\Gamma(\mu+\nu+\lambda+1/2)}{\Gamma(\nu+1/2)\Gamma(\mu+\nu+\lambda+2)} \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+1)} D^{2\nu},$$

$$Q_4(\mu, \nu) = G_3(\mu, \nu) \\ \times \frac{(-1)^{\mu+\nu}\Gamma(\mu-\nu+\lambda+2)}{\Gamma(\nu-\mu-\lambda-3/2)\Gamma(-\nu+3/2)} \left(\frac{k}{2}\right)^{2\nu} \\ \times D^{2(\nu-\mu-\lambda-3/2)},$$

$$Q_5(\mu, \nu) = G_3(\mu, \nu) \\ \times \frac{(-1)^{\lambda+1}\psi_3(\mu, \nu)}{\Gamma(\mu+\nu+\lambda+3)\Gamma(\nu+1/2)\Gamma(-\mu-\nu-\lambda-1/2)} \\ \times \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+2)} D^{2\nu+1},$$

$$Q_6(\mu, \nu) = G_3(\mu, \nu) \\ \times \frac{(-1)^{\mu+\nu}\Gamma(\mu+\nu+\lambda+3/2)}{\Gamma(\nu+3/2)\Gamma(\mu+\nu+\lambda+3)} \\ \times \left(\frac{k}{2}\right)^{2(\mu+\nu+\lambda+2)} D^{2\nu+1},$$

$$G_1(\mu, \nu) = \frac{1}{\Gamma(\mu+1)\Gamma(\mu+m+2)\Gamma(\nu+1)},$$

$$G_2(\mu, \nu) = \frac{\Gamma(2\mu+2\lambda+3)}{\Gamma(\mu+1)\Gamma(\mu+m+2)\Gamma(\mu+n+2)\Gamma(\mu+2\lambda+3)\Gamma(\nu+1)},$$

$$G_3(\mu, \nu) = \frac{\Gamma(2\mu+2\lambda+4)}{\Gamma(\mu+1)\Gamma(\mu+m+2)\Gamma(\mu+n+2)\Gamma(\mu+2\lambda+4)\Gamma(\nu+1)},$$

$$\psi_1(\mu, \nu) = -\psi(\nu+1) - \psi(\mu+\nu+\lambda+2) - \psi(\nu+n+2) \\ + \psi(-\mu-\nu-\lambda+1/2) + 2 \log(k/2),$$

$$\psi_2(\mu, \nu) = -\psi(\nu+1) - \psi(\mu+\nu+\lambda+2) - \psi(\nu+\frac{1}{2}) \\ + \psi(-\mu-\nu-\lambda+1/2) + 2 \log(kD/2),$$

$$\psi_3(\mu, \nu) = -\psi(\nu+1) - \psi(\mu+\nu+\lambda+3) - \psi(\nu+\frac{1}{2}) \\ + \psi(-\mu-\nu-\lambda-1/2) + 2 \log(kD/2),$$

and

$$\psi(x) = \partial \log \Gamma(x) / \partial x.$$

4. TRANSMISSION COEFFICIENT

The transmission coefficient is given by⁶

$$t = \frac{\text{Im} \left(\int_{-a}^{-a-2} \phi^*(x, 0) \partial \phi(x, 0) / \partial z dx \right)}{\text{Im} \left(\int_{-a-2}^{-a} \phi_0^*(x, 0) \partial \phi_0(x, 0) / \partial z dx \right)}, \quad (40)$$

where the asterisk indicates the complex conjugate. Assuming that the function $w(x)$ and $u_n(x)$ are real, we have by Eqs. (8), (11), and (13)

$$\phi^*(x, 0) = 2\pi \sum_{n=0}^{\infty} [A_n^* w(x_1) u_n(x_1) + B_n^* w(x_2) u_n(x_2)] \\ (|x_1| < 1, |x_2| < 1). \quad (41)$$

TABLE I. Plane wave transmission coefficients t of two slits for normal incidence (k : wavenumber, D : distance between slits).

k	$t(D=3)$	$t(D=4)$	$t(D=6)$	$t(D=10)$	$t(D=\infty)$
0.2	0.00586	0.00541	0.00487	0.00387	0.00262
0.4	0.04910	0.04103	0.03055	0.02192	0.02392
0.6	0.15437	0.11738	0.08716	0.08702	0.09484
0.8	0.31068	0.24173	0.22697	0.27763	0.26059
1.0	0.50912	0.45359	0.56886	0.53911	0.54540
1.2	0.74825	0.78565	0.99005	0.88710	0.87693
1.4	0.98583	1.18460	1.11409	1.14506	1.11719
1.6	1.16595	1.37724	1.20077	1.21146	1.21668
1.8	1.26098	1.29857	1.22779	1.23178	1.22129
2.0	1.25712	1.18083	1.20493	1.18792	1.18426
2.5	1.06815	1.04923	1.05536	1.06670	1.06380
3.0	0.96158	0.97605	0.97431	0.97260	0.97202

From Eqs. (4), (7), and (18)

$$\frac{\partial \phi(x, 0)}{\partial z} = \frac{\partial \phi_0(x, 0)}{\partial z} = \begin{cases} -\sum_{m=0}^{\infty} F_m^{(1)} u_m(x_1) & |x_1| < 1, \\ \sum_{m=0}^{\infty} F_m^{(2)} u_m(x_2) & |x_2| < 1. \end{cases} \quad (42)$$

Substitution of Eqs. (41) and (42) into Eq. (40) yields

$$t = -2\pi \frac{\text{Im} \sum_{m=0}^{\infty} (A_m^* F_m^{(1)} + B_m^* F_m^{(2)})}{\text{Im} (J_{-a/2} + J_{a/2}) \phi_0^*(x, 0) f(x) dx}. \quad (43)$$

For a case of normal incidence of a plane wave,

$$\phi_0 = \exp(ikz) \text{ and } f(x) = ik. \quad (44)$$

We find from Eqs. (19), (25), (28), and (29)

$$F_0^{(1)} = F_0^{(2)} = -ik(\pi/2)^{1/2} \text{ and } F_m^{(1)} = F_m^{(2)} = 0 \quad (m \geq 1). \quad (45)$$

Hence we obtain

$$t = (\pi/2)^{3/2} \text{Re}(A_0 + B_0). \quad (46)$$

Numerical values of t calculated from Eq. (46) are given in Table I for $D=3, 4, 6, 10$, and ∞ , where we solve a finite set of equations

$$\sum_{n=0}^9 (P_{mn} A_n + Q_{mn} B_n) = F_m^{(1)} \quad (m=0, 1, 2, \dots, 9),$$

$$\sum_{n=0}^9 (Q_{nm} A_n + P_{nm} B_n) = F_m^{(2)} \quad (m=0, 1, 2, \dots, 9),$$

instead of Eqs. (20) and (23).

5. DISCUSSION

Our method consists of reducing the boundary value problem to a pair of infinite sets of linear algebraic equations and solving it. On these procedures we note the following, which require further investigations: (a) The coefficients of the infinite sets of equations are given by Eqs. (32) and (33), which contain integrals over Bessel functions. These integrals are evidently convergent for any values of parameters and can be computed by numerical integration. In this paper we use the series representations (36)–(39) for the coefficients, which are expected to converge for all values of k and D . Though rigorous proof is not given, the derivation of these series from their integral

forms supports this conjecture. (b) We examine the rate of convergence of Eqs. (36)–(39) by numerical computation. As may be expected, the rate of convergence is good for small values of k and D only. For $k=3$ and $D=10$, for example, we need to set $0 \leq \mu, \nu \leq 60$ to obtain eight significant figures of the result. The values of the coefficients are checked by hand and by numerical integration of Eqs. (32) and (33). (c) We have not been able to prove that the infinite set of equations has a unique solution. What we do in this paper is to solve the truncate set of equations

$$\sum_{n=0}^N (P_{mn} A_n + Q_{mn} B_n) = F_m^{(1)} \quad (m=0, 1, 2, \dots, N),$$

$$\sum_{n=0}^N (Q_{nm} A_n + P_{nm} B_n) = F_m^{(2)} \quad (m=0, 1, 2, \dots, N),$$

numerically. We calculate the solutions A_n and B_n for different values of N and observe that their values converge rapidly as N increases. In the range of k and D in Table I, $N=9$ is enough to obtain eight significant figures.

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APPENDIX

(1) We consider the integral

$$I = \int_0^{\infty} (s^2 - k^2)^{1/2} [J_{\alpha}(s) J_{\beta}(s) / s^{\gamma}] ds,$$

where $a \geq 1$, $\beta \geq 1$, and $\gamma \geq 2$. Separating it into real and imaginary parts, we have $I = I_1 - iI_2$, where

$$I_1 = \int_k^{\infty} (s^2 - k^2)^{1/2} [J_{\alpha}(s) J_{\beta}(s) / s^{\gamma}] ds$$

and

$$I_2 = \int_0^k (k^2 - s^2)^{1/2} [J_{\alpha}(s) J_{\beta}(s) / s^{\gamma}] ds.$$

The radiation condition requires that $\arg(-1)^{1/2} = 3\pi/2$ throughout this paper. To evaluate the integral I_1 , we introduce the representations

$$J_{\alpha}(s) = \sum_{\mu=0}^{\infty} \frac{(-1)^{\mu}}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)} \left(\frac{s}{2}\right)^{2\mu+\alpha} \quad (A1)$$

and

$$J_{\beta}(s) = \frac{1}{2\pi i} \int_{-c-i\infty}^{-c+i\infty} \frac{\Gamma(-h)}{\Gamma(h+\beta+1)} \left(\frac{s}{2}\right)^{2h+\beta} dh \quad (c > 0), \quad (A2)$$

and obtain

$$I_1 = \frac{1}{2\pi i} \sum_{\mu=0}^{\infty} \frac{(-1)^{\mu}}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)} \left(\frac{1}{2}\right)^{2\mu+\alpha+\beta}$$

$$\times \int_{-c-i\infty}^{-c+i\infty} dh \frac{\Gamma(-h)}{\Gamma(h+\beta+1)} \left(\frac{1}{2}\right)^{2h}$$

$$\times \int_k^{\infty} (s^2 - k^2)^{1/2} s^{2\mu+2h+\alpha+\beta-\gamma} ds.$$

Using the formula

$$\int_k^{\infty} (s^2 - k^2)^{1/2} s^{\rho} ds = \frac{\pi^{1/2} \Gamma(-\rho/2 - 1)}{4\Gamma(-\rho/2 + 1/2)} k^{\rho+2} \quad (\text{Re } \rho < -2) \quad (A3)$$

and setting $\alpha + \beta - \gamma = 2\lambda$ ($\lambda = 0, 1, 2, \dots$), we have

$$I_1 = \frac{k^{2\lambda+2}}{8\pi^{1/2}i} \left(\frac{1}{2}\right)^{\alpha+\beta} \sum_{\mu=0}^{\infty} \frac{(-1)^\mu}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)} \left(\frac{k}{2}\right)^{2\mu} \\ \times \int_{-c-i\infty}^{-c+i\infty} \frac{\Gamma(-h)\Gamma(-h-\mu-\lambda-1)}{\Gamma(h+\beta+1)\Gamma(-h-\mu-\lambda+1/2)} \left(\frac{k}{2}\right)^{2h} dh \\ (c > \mu + \lambda + 1).$$

Straightforward calculation of residues yields the result.

The integral I_2 is similarly evaluated by using the formula

$$\int_0^k (k^2 - s^2)^{1/2} s^p ds = \frac{\pi^{1/2} \Gamma(p/2 + 1/2)}{4\Gamma(p/2 + 2)} k^{p+2} \\ (\text{Re } p > -1), \quad (\text{A4})$$

instead of Eq. (A3).

(2) The integrals

$$J = \int_0^\infty (s^2 - k^2)^{1/2} \frac{J_\alpha(s)J_\beta(s)}{s^\gamma} \begin{cases} \cos Ds \\ \sin Ds \end{cases} ds$$

are also evaluated by the same procedure, where we employ the formulas

$$J_\alpha(s)J_\beta(s) \\ = \sum_{\mu=0}^{\infty} \frac{(-1)^\mu \Gamma(2\mu + \alpha + \beta + 1)}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)\Gamma(\mu+\beta+1)\Gamma(\mu+\alpha+\beta+1)} \\ \times \left(\frac{s}{2}\right)^{2\mu+\alpha+\beta}, \quad (\text{A5})$$

$$\cos Ds = (\pi Ds/2)^{1/2} J_{-1/2}(Ds), \quad \sin Ds = (\pi Ds/2)^{1/2} J_{1/2}(Ds), \\ (\text{A6})$$

and Eq. (A2).

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ERRATA

Erratum: Asymmetric gas thermodynamics [*J. Math. Phys.* **18**, 858 (1977)]

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Now that the reprints of the above paper have been sent out to various colleagues around the world, it has been kindly brought into my attention that one term is missing from four equations in the above paper. These are:

(1) $\epsilon_{ikl} \tau_{kl} \omega_i$ should be added on the lhs of Eq. (2.4)

and on the lhs of inequality (2.16), inside the last parenthesis.

(2) $\Lambda \epsilon_{ikl} \tau_{kl} \omega_i$ should be added on the lhs of inequality (2.28) and on the lhs of inequality (2.29); everything else remains unchanged.

and setting $\alpha + \beta - \gamma = 2\lambda$ ($\lambda = 0, 1, 2, \dots$), we have

$$I_1 = \frac{k^{2\lambda+2}}{8\pi^{1/2}i} \left(\frac{1}{2}\right)^{\alpha+\beta} \sum_{\mu=0}^{\infty} \frac{(-1)^\mu}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)} \left(\frac{k}{2}\right)^{2\mu} \\ \times \int_{-c-i\infty}^{-c+i\infty} \frac{\Gamma(-h)\Gamma(-h-\mu-\lambda-1)}{\Gamma(h+\beta+1)\Gamma(-h-\mu-\lambda+1/2)} \left(\frac{k}{2}\right)^{2h} dh \\ (c > \mu + \lambda + 1).$$

Straightforward calculation of residues yields the result.

The integral I_2 is similarly evaluated by using the formula

$$\int_0^k (k^2 - s^2)^{1/2} s^p ds = \frac{\pi^{1/2} \Gamma(p/2 + 1/2)}{4\Gamma(p/2 + 2)} k^{p+2} \\ (\text{Re } p > -1), \quad (\text{A4})$$

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$$J_\alpha(s)J_\beta(s) \\ = \sum_{\mu=0}^{\infty} \frac{(-1)^\mu \Gamma(2\mu + \alpha + \beta + 1)}{\Gamma(\mu+1)\Gamma(\mu+\alpha+1)\Gamma(\mu+\beta+1)\Gamma(\mu+\alpha+\beta+1)} \\ \times \left(\frac{s}{2}\right)^{2\mu+\alpha+\beta}, \quad (\text{A5})$$

$$\cos Ds = (\pi Ds/2)^{1/2} J_{-1/2}(Ds), \quad \sin Ds = (\pi Ds/2)^{1/2} J_{1/2}(Ds), \\ (\text{A6})$$

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