The bounding properties of the multipoint Padé approximant to a series of Stieltjes on the real line*

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(Received 12 June 1972; revised manuscript received 3 October 1972)

The multipoint Padé approximants to a series of Stieltjes and the corresponding complementary approximants are defined. Their bounding properties are established, and those of the usual $[n,n-1]$ and $[n,n]$ Padé approximants are shown to be special cases. It is further shown how information in the form of the first few terms in the expansion of the series of Stieltjes in inverse powers of x may be incorporated into the multipoint Padé approximant and its complement, thereby tightening the bounds supplied by the approximants. The usual "two-point" Padé approximant occurs as a special case of following this procedure. Physically occurring series of Stieltjes can often be written in the form $G(x) = \sum_{k=1}^{K} V_k/(\mathcal{E}_k + x) + H(x)$, where $G(x)$ is a series of Stieltjes with radius of convergence $R > 0$, $H(x)$ is a series of Stieltjes with radius of convergence $R' > R$, $R \leq \mathcal{E}_1 < \mathcal{E}_2 < \ldots < \mathcal{E}_K < R'$, and $0 < V_k < \infty$ $(k=1,2,\ldots,K)$. In addition to the bounds supplied by the multipoint Padé approximants for $X \in (-R, \infty)$, it is shown that the approximants also exhibit interesting bounding properties for $X \in (-R', -R)$. A theorem on these bounding properties is proved. It is further shown that the multipoint Padé approximants yield best possible upper bounds on the $\mathcal{E}_k$ and on V_1, but, in general, do not yield straightforward bounds on $V_2, V_3, \ldots, V_K$. Finally, the effect of fixing the locations of the poles of the multipoint Padé approximant and its complement at the correct values $x=-\mathcal{E}_k$ $(k=1, 2, \ldots, K)$ is considered. The resulting approximants then impose a complementary pair of bounds on $G(x)$ for $-R' < x < \infty$, which in most cases will be the best possible. In particular, one can now usually obtain best possible upper and lower bounds on $V_1, V_2, \ldots, V_K$.

1. INTRODUCTION

In view of the current interest in, and usage of, the one- and two-point Padé approximant method as a means for analytically continuing and bounding functions with physical significance,[1-3] it appears relevant that the bounding properties on the real line of the general multipoint Padé approximant to a series of Stieltjes be stated and proved. So far as this author knows these results have not been explicitly set down before. By a series of Stieltjes we mean any *function* which may be *represented* by a series of Stieltjes (thus being the analytic continuation of that series).

In Secs. 2, 3, and 4, the bounding properties of the approximants when $-R < x \leq \infty$, where R is the radius of convergence of the series of Stieltjes, are presented in a unified manner, thereby displaying the bounding properties of the usual $[n, n-1]$ and $[n, n]$ one-point Padé approximants as a special case. It is believed that such a presentation will help to make the many possible applications of this theory to physical problems more apparent. The derivation of these results is based on an earlier paper by Baker[4] (hereafter referred to as GB), and could have been obtained from a moment theoretical approach.[5] However, it is believed that the statement of these results made in the context of the Padé approximant approach has the advantage that it highlights the important fact that the multipoint Padé approximants achieve the approximate analytic continuation for the large class of functions being considered, using information about the function in a limited region. In fact, the approximants use the first few terms from each of a *set* of power series expansions of the "series of Stieltjes" function under consideration. Even if all the terms in these power series had been known, their radii of convergence would all be bounded. The approximants not only impose best possible bounds on the function both inside and *outside* the region of convergence of the set of power series involved, but also reproduce the function inside the region of convergence more accurately than the known terms of any of the individual series.

The results of the first sections can also be derived variationally,[6] taking as a starting point a Hylleraas variational principle used by Epstein[7] to obtain the usual one-point Padé approximants for the dynamical polarizability (see below). Such an approach has the advantages of elegance, and for those who like to think variationally (for example, theoretical chemists), of clarity.

In Sec. 5 further results are presented, some of which are new even to the theory of the usual $[n, n-1]$ and $[n, n]$ one-point Padé approximants. These pertain to the bounding properties of the multipoint Padé approximants *within* the region of poles $-\infty < x < -R$. They apply when the function being approximated is of the special but frequently occurring form

$$G(x) = \sum_{k=1}^{K} \frac{V_k}{(\mathcal{E}_k + x)} + H(x),$$

where $G(x)$ is a series of Stieltjes with radius of convergence $R > 0$, $H(x)$ is a series of Stieltjes with radius of convergence $R' > R$, $R \leq \mathcal{E}_1 < \mathcal{E}_2 < \cdots < \mathcal{E}_K < R'$ and $0 < V_k < \infty$ $(k = 1, 2, \ldots, K)$. Such a series of Stieltjes is the dynamical polarizability $\alpha(\omega^2)$ for an atom in its ground state.[8] Here ω is a real or imaginary frequency, the V_k correspond to oscillator strengths, and the $\mathcal{E}_k$ to the squares of excitation energies of the atom. The multipoint approximant to this type of function then supplies various bounds on $G(x)$, not only for $-R < x < \infty$, but also for $-R' < x < -R$. Furthermore, best possible upper bounds on $\mathcal{E}_k$ $(k = 1, 2, \ldots, K)$ and on V_1, but not on $V_2, V_3, \ldots, V_K$, can be obtained. Thus, for example, in the case of the dynamical polarizability one could make direct use of refractive index information at low frequency to derive bounds for the refractive index at frequencies *higher* than the first excitation energy of the atom; to derive bounds on some of the excitation energies; and to derive an upper bound to the first oscillator strength.

Finally, in Sec. 6, we consider the effect of incorporating information regarding the locations of the discrete poles of $G(x)$ into the construction of the multipoint Padé approximant and its complement. If the locations of the

first K discrete poles of $G(x)$, $x = -\mathcal{E}_k$ $(k = 1, 2, \ldots, K)$ are known then, by ensuring that the two approximants also have poles at these points, one is able to obtain a complementary pair of bounds on $G(x)$ for $-R' < x < \infty$, and these bounds will be best possible in *most* cases. For $-R' < x < -\mathcal{E}_1$, these bounds are of a definite form as contrasted with the corresponding situation, discussed in Sec. 5, in which the locations of the poles of $G(x)$ are not known. In particular, one can now usually obtain best possible upper and lower bounds on the pole strengths $V_1, V_2, \ldots, V_K$.

In general, the multipoint Padé approximant method is applicable *in some sense* whenever a set of information (functional values, asymptotic behavior, etc.) is available for a physical function $P(z)$, assumed to be well behaved throughout most of the complex plane. Multipoint approximants constructed on the basis of the given information are often assumed to represent or echo in some way the behavior of $P(z)$ *throughout* the complex plane.[1] In particular the approximant is considered to approximate the functional values of $P(z)$, and the singularities of the approximant to correspond somehow to the singularities of $P(z)$. A current problem[9] in approximation theory is the determination of conditions under which rigorous statements can be made regarding the relationship between $P(z)$ and multipoint Padé approximants[10] to it. By examining in detail the relationship between the multipoint approximants and the series of Stieltjes which they approximate in the *region of poles*, it is hoped that further insight into the general problem of rational approximation will be obtained.

2. THE N/P PADÉ APPROXIMANT TO A SERIES OF STIELTJES

Let $F(x)$ be a series of Stieltjes with radius of convergence R. Then $F(x)$ can be written in the form

$$F(x) = \int_0^{1/R} \frac{d\phi(u)}{(1+ux)}, \tag{1}$$

where $\phi(u)$ is a bounded, monotone nondecreasing function, which attains infinitely many values in the interval $0 \leq u < 1/R$. It is easily seen that $F(x)$ is a positive monotone decreasing function for $-R < x < \infty$, and that it is continuous and infinitely differentiable over this interval.

Let $\{x_i\}_{i=1}^{P}$ where $-R < x_1 < x_2 < \cdots < x_P < \infty$ be a set of points corresponding to which the values

$$F^{(n)}(x_m), \quad n = 0, 1, 2, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P \tag{2}$$

are known, where $F^{(n)}(x_m)$ denotes the nth derivative of $F(x)$ evaluated at x_m. If

$$\sum_{m=1}^{P} N_m = N,$$

then we will say that we have N *pieces of information about* $F(x)$ at P *points*. Thus, for example, if we know

$$F(x_m), \quad m = 1, 2, \ldots, P,$$

then we have P pieces of information about $F(x)$ at P points.

The multipoint Padé approximant to $F(x)$ associated with such a set of given information (2) is the function

$$f_{N(P)}(x) = A_N(x)/B_N(x),$$

where $A_N(x)$ and $B_N(x)$ are *the* polynomials of degrees $[(N-1)/2]$ and $[N/2]$, respectively, which are uniquely determined by the conditions

$$f_{N(P)}^{(n)}(x_m) = F^{(n)}(x_m), \quad n = 0, 1, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P$$

together with a normalization requirement

$$B_N(0) = 1.$$

Throughout we use the notation $[y]$ to mean the integer part of y. We notice that there are $(N+1)$ unknowns involved in the two polynomials which constitute the approximant, and that we have precisely this number of equations for their determination.

The uniqueness of such an approximant is easily established by considering the difference between two such approximants which satisfy the same set of conditions. The existence of the approximant is established in GB, being assured because the given information relates to a series of Stieltjes: if the given information had been specified in an entirely *arbitrary* fashion then existence would not be guaranteed.[11] In fact, in the case of P points and P pieces of information, the existence of the approximant is easily established if one result (proved in GB) is accepted here without proof. If $F(x)$ is a series of Stieltjes with radius of convergence R, then $F_1(x)$ defined by

$$F(x) = F(x_1)/[1 + (x - x_1)F_1(x)], \quad \text{any } x_1 \in (-R, \infty)$$

is also a series of Stieltjes, but with radius of convergence *at least* R. Thus, in general, if $-R < x_1 < x_2 < \cdots < x_P < \infty$, then $F_P(x)$ defined by

$$F(x) = \cfrac{a_1}{1 + (x - x_1)a_2 \Big/ \left(1 + \cdots \Big/ \left(1 + \cfrac{(x - x_{P-1})a_P}{1 + (x - x_P)F_P(x)}\right)\right)} \tag{3}$$

will be a series of Stieltjes with radius of convergence at least R providing $a_1, a_2, \ldots, a_P$ can be chosen so that both sides of (3) agree at $x_1, x_2, \ldots, x_P$. That they can be thus chosen is assured by using the successive scheme

$$F_0(x) = F(x),$$
$$F_n(x) = [F_{n-1}(x_n) - F_{n-1}(x)]/(x - x_n)F_{n-1}(x), \quad 1 \leq n \leq P,$$
$$a_n = F_{n-1}(x_n),$$

and noting that each $F_n(x)$ is a series of Stieltjes with radius of convergence at least R so that each $a_n > 0$ (the scheme would break down if any of the a_n could have vanished). If we now set $F_P(x) \equiv 0$, then the right-hand side of (3) becomes precisely the approximant whose existence we sought to demonstrate. The existence of the general multipoint Padé approximant to a series of Stieltjes is established in GB by using similar arguments. We will refer to the general multipoint Padé approximant as an $N(P)$ approximant.

The bounding properties of the general $N(P)$ approximant, with respect to a series of Stieltjes, can be deduced easily once the bounding properties of a $P(P)$ approximant are established.

To achieve the latter we consider the difference

$$F(x) - f_{P(P)}(x) = \frac{a_1}{1 + (x-x_1)a_2 \Big/ 1 + \ddots \dfrac{(x-x_{P-1})a_P}{1+(x-x_P)F_P(x)}} - \frac{a_1}{1 + (x-x_1)a_2 \Big/ 1 + \ddots \dfrac{(x-x_{P-1})a_P}{1+0}}.$$

Suppose, for example, that $-R < x < x_1$. Then

$$0 < \frac{a_P}{1+0} < \frac{a_P}{1+(x-x_P)F_P(x)} = F_{P-1}(x),$$

where the positivity of a_P is used, and the term on the right is guaranteed to be positive because $F_{P-1}(x)$ is a series of Stieltjes with radius of convergence at least R. Hence

$$0 < \frac{a_{P-1}}{1 + (x-x_{P-1})a_P \Big/ 1+0} < \frac{a_{P-1}}{1 + (x-x_{P-1})a_P \Big/ 1+(x-x_P)F_P(x)} = F_{P-2}(x)$$

and so on until finally we obtain

$$0 < f_{P(P)}(x) < F(x) \text{ for } -R < x < x_1.$$

Similar reasoning applies to each of the intervals $x_1 < x < x_2, x_2 < x < x_3, \ldots, x_P < x < \infty$, and we find that

$$\begin{aligned} &0 < F(x) < f_{P(P)}(x) && \text{for } x_1 < x < x_2 \\ &0 < f_{P(P)}(x) < F(x) && \text{for } x_2 < x < x_3 \\ &\quad \cdots && \quad \cdots \\ &\left.\begin{matrix} 0 < f_{P(P)}(x) < F(x) \\ \text{or} \\ 0 < F(x) < f_{P(P)}(x) \end{matrix}\right\} && \text{for } x_P < x < \infty. \end{aligned}$$

It is now a simple matter to deduce the bounds imposed by the general $N(P)$ approximant on $F(x)$. We need only note that an $f_{N(P)}(x)$ can always be realized as a limiting case of an $f_{N(N)}(x)$. We start with an $f_{N(N)}(x)$ and let the first N_1 points $x_1, x_2, \ldots, x_{N_1}$ tend to coincidence at x_1, then let the next N_2 points tend to coincidence at x_2, and so on until we finally obtain the requisite $f_{N(P)}(x)$. The bounds imposed by the resulting approximant (which of course is not constructed in this way[12]) are then seen immediately. As an example we have sketched the bounding relationship between an $f_{4(3)}(x)$ and $F(x)$ in Fig. 1. The directions of the bounds are a direct consequence of the relationship between $f_{4(4)}(x)$ and $F(x)$, as sketched in Fig. 2.

The well known bounding properties of the usual $[[N/2], [(N-1)/2]]$ Padé approximants,[13,14] which use N pieces of information at one point $x = 0$, are immediate when one observes that in this case

$$[[N/2], [(N-1)/2]] = f_{N(1)}(x).$$

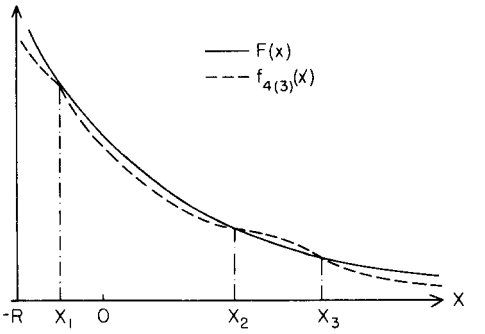

FIG. 1. Sketch illustrating the bounding relationship between $F(x)$ and a typical 4(3) multipoint Padé approximant to it. Here the given information is $F(x_i)$ $(i = 1, 2, 3)$ and $F^{(1)}(x_1)$, with $-R < x_1 < 0 < x_2 < x_3 < \infty$. The bounds supplied by $f_{4(3)}(x)$ may be viewed as a limiting case of those supplied by an $f_{4(4)}(x)$ as illustrated in Fig. 2.

3. THE COMPLEMENTARY $N(P)$ PADÉ APPROXIMANT TO A SERIES OF STIELTJES

By explicitly making use of the one additional piece of information that $F(x)$ is a series of Stieltjes with *radius of convergence (at least)* R, bounds which are precisely complementary to those supplied by the $N(P)$ approximant can be obtained. To see this we again consider the case where P pieces of information at P points is given. In this case it is shown in GB that (3) can be multiplied up to yield

$$F(x) = \frac{B_{P-1}(-R)A_P(x) + (x-x_P)\tilde{F}_P(x)B_P(-R)A_{P-1}(x)}{B_{P-1}(-R)B_P(x) + (x-x_P)\tilde{F}_P(x)B_{P-1}(x)B_P(-R)}, \tag{4}$$

where $\tilde{F}_P(x) = C_P F_P(x)$, C_P being a positive constant, and where the polynomials $A_{P-1}(x), B_{P-1}(x)$ correspond to the $f_{(P-1)(P-1)}(x)$ which uses the information at the first $(P-1)$ points, $x_1, x_2, \ldots, x_{P-1}$. Further, it is shown in GB that the range of possible values attainable by $F(x)$ for any fixed $x \in (-R, \infty)$ is given by the map under (4) of the interval

$$0 < \tilde{F}_P(x) < (R + x_P)^{-1}.$$

If we now take the derivative of F with respect to $\tilde{F}_P$ we find

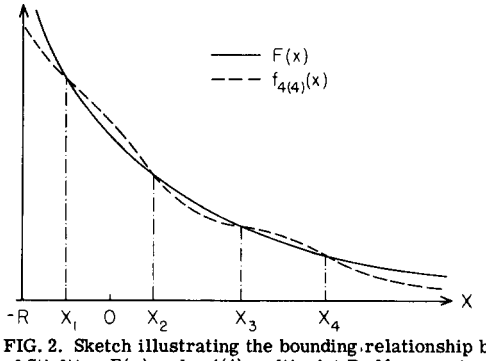

FIG. 2. Sketch illustrating the bounding relationship between a series of Stieltjes $F(x)$ and a 4(4) multipoint Padé approximant to it, for $-R < x < \infty$. $F(x)$ has radius of convergence R, and the given information is $F(x_i)$ $(i = 1, 2, 3, 4)$ with $-R < x_1 < 0 < x_2 < x_3 < x_4 < \infty$.

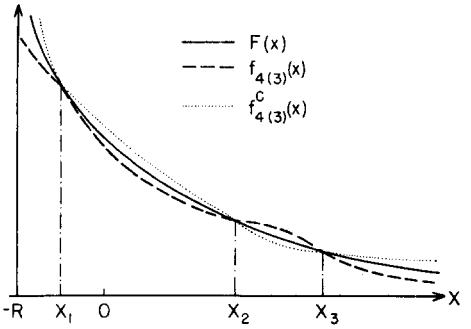

FIG. 3. Sketch illustrating the bounding relationship between $F(x)$, a multipoint Padé approximant $f_{4(3)}(x)$ to it, and the corresponding complementary multipoint Padé approximant $f^C_{4(3)}(x)$. The information used to construct the approximants is $F(x_i)(i = 1, 2, 3)$, $F^{(1)}(x_1)$, where $-R < x_1 < 0 < x_2 < x_3 < \infty$, and $F(x)$ is known to have a radius of convergence (at least) R.

$$\frac{dF}{d\tilde{F}_P} = \frac{B_P(-R)B_{P-1}(-R)B_{P-1}(x)B_P(x)}{[B_{P-1}(-R)B_P(x) + (x-x_P)\tilde{F}_P(x)B_{P-1}(x)B_P(-R)]^2} \times (x-x_P)[A_P(x)/B_P(x) - A_{P-1}(x)/B_{P-1}(x)]$$

Here, both the denominator and the factor[15] $B_P(-R)B_{P-1}(-R)B_{P-1}(x)B_P(x)$ are positive for $x \in (-R, \infty)$, and hence the sign of the derivative is dependent only on the factor $(x-x_P)[A_P(x)/B_P(x) - A_{P-1}(x)/B_{P-1}(x)]$. Since $A_{P-1}(x)/B_{P-1}(x)$ is not only the $(P-1)(P-1)$ approximant to $F(x)$, corresponding to information at the first $(P-1)$ points, $x_1, x_2, \ldots, x_{P-1}$, but also the $(P-1)(P-1)$ approximant to $f_{P(P)}(x) = A_P(x)/B_P(x)$, we see that the sign of the derivative $dF/d\tilde{F}_P$ changes exactly P times for $x \in (-R, \infty)$, one sign change occurring at each of the points $x_1, x_2, \ldots, x_P$. In particular, on each of the intervals $(-R, x_1), (x_1, x_2), \ldots, (x_P, \infty)$, the value of F is monotonically dependent on the value of $\tilde{F}_P$, either increasing or decreasing. Thus, the *best possible* bounds that can be imposed on $F(x)$ for $x \in (-R, \infty)$ are supplied by the two approximants obtained by setting $\tilde{F}_P \equiv 0$ and $\tilde{F}_P \equiv (R + x_P)^{-1}$ in the right-hand side of (4). Further, the resulting bounds will be complementary: When one approximant supplies an upper bound the other must supply a lower bound, and vice-versa. Setting $\tilde{F}_P \equiv 0$ we reobtain the $P(P)$ approximant

$$f_{P(P)}(x) = A_P(x)/B_P(x), \tag{5}$$

and we deduce that its previously established bounding properties are best possible. Setting $\tilde{F}_P(x) \equiv (R + x_P)^{-1}$, we obtain the complementary approximant

$$f^C_{P(P)}(x) = \frac{(R+x_P)B_{P-1}(-R)A_P(x) + (x-x_P)B_P(-R)A_{P-1}(x)}{(R+x_P)B_{P-1}(-R)B_P(x) + (x-x_P)B_{P-1}(x)B_P(-R)}$$

whose bounding properties must also be the best possible.

In the general case of N pieces of information at P points, it follows from a limiting argument similar to the one used previously that the bounding properties of $f_{N(P)}(x)$ are best possible, and that the best possible complementary bounds are supplied by

$$f^C_{N(P)}(x) = \frac{(R+x_P)B_{N-1}(-R)A_N(x) + (x-x_P)B_N(-R)A_{N-1}(x)}{(R+x_P)B_{N-1}(-R)B_N(x) + (x-x_P)B_{N-1}(x)B_N(-R)},$$

where the polynomials A_N and B_N now correspond to $f_{N(P)}(x)$, and the polynomials A_{N-1}, B_{N-1} correspond to the $f_{(N-1)(P)}(x)$ or $f_{(N-1)(P-1)}(x)$ which is obtained when the "first" $(N-1)$ pieces of information are used. An example of the bounding relationship between an $f_{N(P)}(x)$, $f^C_{N(P)}(x)$, and $F(x)$ is sketched in Fig. 3.

Having established the existence and bounding properties of $f^C_{N(P)}(x)$ in the manner described above, we now observe that the complementary approximant is unique and hence it is most easily obtained as follows: We set

$$f^C_{N(P)}(x) = C_N(x)/D_N(x),$$

where $C_N(x)$ and $D_N(x)$ are *the* polynomials of degrees $[N/2]$ and $[(N+1)/2]$, respectively, which are uniquely specified by the set of conditions

$$(f^C_{N(P)})^{(n)}(x_m) = F^{(n)}(x_m), \quad n = 0, 1, 2, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P$$

together with the requirements

$$D_N(0) = 1 \quad \text{and} \quad D_N(-R) = 0.$$

The latter condition serves to place a pole of the approximant at $x = -R$. We note that there are now $(N+2)$ unknowns involved in the two polynomials which constitute the approximant and that we have precisely this number of equations. Methods for solving this set of equations are similar to those which can be used to obtain $f_{N(P)}(x)$.[12]

In the special case that all the information corresponds to the one point $x = 0$, $f^C_{N(P)}(x)$ reduces to

$$f^C_{N(1)}(x) = \frac{RB_{N-1}(-R)A_N(x) + xB_N(-R)A_{N-1}(x)}{RB_{N-1}(-R)B_N(x) + xB_{N-1}(x)B_N(-R)}.$$

This approximant is precisely the one obtained in GB, and the bounds which it supplies are complementary to those given by the usual $[[N/2], [(N-1)/2]]$ Padé approximant which utilizes the same set of given information.

4. UTILIZATION OF COEFFICIENTS FROM THE SERIES EXPANSION OF $F(x)$ IN INVERSE POWERS OF x

Here we suppose that in addition to the given information (2) we have available the coefficients of the first few terms in the expansion of $F(x)$ in powers of $(1/x)$.

Taking $F(x)$ as in (1), we rewrite

$$F(x) = F_0 + \int_0^{1/R} \frac{d\tilde{\phi}(u)}{(1+ux)} = F_0 + \tilde{F}(x),$$

where $0 \leq F_0 = \lim \int_0^{\epsilon} d\phi(u) < \infty$ as $\epsilon \to 0+$ and where

$$\tilde{\phi}(u) = \begin{cases} \phi(u) & \text{for } 0 < u < 1/R \\ \lim_{u \to 0+} \phi(u) & \text{for } u = 0 \end{cases},$$

so that $\tilde{F}(x)$ is also a series of Stieltjes but such that

$\tilde{F}(x) \to 0$ as $x \to \infty$.

What we suppose here, then, is that in addition to the given information (2) about $F(x)$, we are also told

$$F(x) \sim F_0 + \sum_{j=1}^{J-1} (-1)^{j+1}\left(\frac{1}{x}\right)^j \tilde{F}_{-j} + \begin{cases}\text{terms with unknown}\\ \text{or divergent coef-}\\ \text{ficients}\end{cases}$$

where

$$\tilde{F}_{-j} = \int_0^{1/R} \frac{d\tilde{\phi}(u)}{u^j} \quad (j = 1, 2, \ldots, J-1)$$

are finite numbers. These additional moments can be incorporated into the multipoint Padé approximant and its complement by generalizing a device used by Langhoff and Karplus.[16]

We need only note that the finiteness of the $\tilde{F}_{-j}$'s ($j = 1, 2, \ldots, J-1$) is sufficient to ensure that the function $\eta(u)$ defined by $d\eta(u) = u^{1-J}d\tilde{\phi}(u)$ is an allowable measure in the definition of a series of Stieltjes providing $\phi(u)$ is. Thus

$$E(x) = \int_0^{1/R} \frac{d\tilde{\phi}(u)}{u^{J-1}(1+ux)}$$

is a series of Stieltjes with radius of convergence at least R. In particular we observe that

$$E(x) = \sum_{n=0}^{J-2} (-x)^n \tilde{F}_{n-J+1} + (-x)^{J-1}[F(x) - F_0]. \quad (6)$$

Since we know $F_0, \tilde{F}_{-1}, \ldots, \tilde{F}_{-J+1}$, we can use (6) to transform the set of given information (2) about $F(x)$ into a new set of given information, pertaining now to the series of Stieltjes $E(x)$. In fact, the numbers

$$F^{(n)}(x_m), \quad n = 0, 1, 2, \ldots, N_m - 1,$$

where $x_m \neq 0$ determine

$$E^{(n)}(x_m), \quad n = 0, 1, 2, \ldots, N_m - 1;$$

and if we have N_0 pieces of information pertaining to the behavior of $F(x)$ at $x = 0$, then we can obtain

$$E^{(n)}(0), \quad n = 0, 1, 2, \ldots, J - 2 + N_0.$$

We have effectively $(N + J - 1)$ pieces of information about the series of Stieltjes $E(x)$, and thus we can construct the related multipoint approximant, and its complement, to $E(x)$. Let these be denoted by $\mathcal{E}_{N(P)+J}(x)$ and $\mathcal{E}^C_{N(P)+J}(x)$, respectively. The corresponding approximants to $F(x)$ are then clearly

$$f_{N(P)+J}(x) = \frac{\mathcal{E}_{N(P)+J}(x) - \sum_{n=0}^{J-2} (-x)^n \tilde{F}_{n-J+1}}{(-x)^{J-1}} + F_0 \quad (7)$$

and

$$f^C_{N(P)+J}(x) = \frac{\mathcal{E}^C_{N(P)+J}(x) - \sum_{n=0}^{J-2} (-x)^n \tilde{F}_{n-J+1}}{(-x)^{J-1}} + F_0.$$

The bounding properties of the latter two approximants can now easily be deduced from the bounding properties of $\mathcal{E}_{N(P)+J}(x)$ and its complement with respect to $E(x)$. We find that

$$f_{N(P)+J}(x) > \text{or} < F(x) \text{ according as } f_{N(P)}(x) > \text{or} < F(x)$$

and

$$f^C_{N(P)+J}(x) > \text{or} < F(x) \text{ according as } f^C_{N(P)}(x) > \text{or} < F(x).$$

Since $\mathcal{E}_{N(P)+J}(x)$ imposes best possible bounds on $E(x)$, it follows that the bounds supplied by $f_{N(P)+J}(x)$ are also best possible, and similarly for their complements (however, see Sec. 6). Thus the inclusion of the additional information simply has the effect of tightening the bounds on $F(x)$; the bounding relationship between $f_{N(P)+J}(x), f^C_{N(P)+J}(x)$, and $F(x)$ is the same as that between $f_{N(P)}(x), f^C_{N(P)}(x)$, and $F(x)$.

In practice, the transformation of the given information (2) under (6) and the subsequent construction of the approximants as described in (7) is unnecessarily cumbersome. Such a procedure has been used here solely for the purpose of establishing the existence and the nature of the bounding properties of the approximants. The uniqueness of the approximants allows us to formulate their construction as follows: We set

$$f_{N(P)+J}(x) = A(x)/B(x) + F_0,$$

where $A(x)$ and $B(x)$ are *the* polynomials of degrees $[(N + J - 3)/2]$ and $[(N + J - 1)/2]$, respectively, which are uniquely specified from the sets of conditions

$$f^{(\eta)}_{N(P)+J}(x_m) = F^{(n)}(x_m), \quad n = 0, 1, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P$$

together with the requirements

$$\tilde{f}_{-j} = \tilde{F}_{-j}, \quad j = 1, 2, \ldots, \begin{cases} J-1 \text{ if } N+J \text{ is } odd \\ J-2 \text{ if } N+J \text{ is } even \end{cases} \quad (8)$$

and a normalization condition

$$B(0) = 1.$$

Here $\tilde{f}_{-j}$ denotes the coefficient of $(1/x)^j$ in the expansion of $f_{N(P)+J}(x)$ in powers of $(1/x)$. The set of equations (8) can be linearized in much the same way as those relating to information at finite points (see Ref. 12).

A similar formulation describes the corresponding complementary approximant. In this case we set

$$f^C_{N(P)+J}(x) = C(x)/D(x) + F_0,$$

where $C(x)$ and $D(x)$ are now of degrees $[(N + J - 2)/2]$ and $[(N + J)/2]$, respectively. The conditions for their determination are similar to those given above, except that now we require

$$\tilde{f}^C_{-j} = \tilde{F}_{-j}, \quad j = 1, 2, \ldots \begin{cases} J-1 \text{ if } N+J \text{ is } even \\ J-2 \text{ if } N+J \text{ is } odd \end{cases},$$

and we have the additional stipulation that

$$D(-R) = 0.$$

We notice that either $f_{N(P)+J}(x)$ or $f^C_{N(P)+J}(x)$, but not

both, fails to utilize the "last" given coefficient $\tilde{F}_{-(J-1)}$. The reason for this can be seen as follows: If $F_0 \neq 0$, then since we must have

$$\lim_{x\to\infty} f_{N(P)+J}(x) = \lim_{x\to\infty} f^C_{N(P)+J}(x) = F_0$$

the degrees of the polynomials in the numerator and denominator of either approximant, expressed in rational form, must be equal. Hence, for one of the approximants, there is necessarily insufficient parameters to allow all of the given information to be matched. If $F_0 = 0$, then, for both approximants, the degree of the polynomial in the denominator must exceed that of the polynomial in the numerator by unity, and again we have the same situation. (If the difference in degrees was greater than unity then the approximant could not be represented as the limiting form of a series of Stieltjes and thus could not have concluded that its bounding properties were best possible.)

In the special case that the given information consists of N pieces of information at the single point $x = 0$, together with J pieces of information pertaining to the behavior of $F(x)$ as $x \to \infty$, we see that $f_{N(1)+J}(x)$ is the "usual" two-point Padé approximant.[1,2,16]

5. BOUNDING PROPERTIES OF THE MULTIPOINT PADÉ APPROXIMANTS IN THE REGION OF THE POLES

In this section we will ultimately be concerned with those series of Stieltjes which have the special but frequently occurring form

$$G(x) = \sum_{k=1}^{K} \frac{V_k}{\mathcal{E}_k + x} + H(x), \tag{9}$$

Here $G(x)$ is a series of Stieltjes with radius of convergence at least $R > 0$, $H(x)$ is a series of Stieltjes with radius of convergence at least R' where $R' > R$, $0 < V_k < \infty$ $(k = 1, 2, \ldots, K)$ and $R \leq \mathcal{E}_1 < \mathcal{E}_2 < \ldots < \mathcal{E}_K < R'$.

We will eventually show that the multipoint approximant $g_{N(P)}(x)$ to $G(x)$, constructed as before, imposes various bounds on $G(x)$ in the region $x \in (-\mathcal{E}_K, -\mathcal{E}_{K-1}) \cup (-\mathcal{E}_{K-1}, -\mathcal{E}_{K-2}) \cup \cdots \cup (-\mathcal{E}_2, -\mathcal{E}_1)$ which we refer to as the *region of poles of* $G(x)$. Further, we will establish that $g_{N(P)}(x)$ yields best possible upper bounds to $\mathcal{E}_m$ $(m = 1, 2, \ldots, \min\{K, [N/2]\})$ and a best possible upper bound to V_1, but not, in general, to $V_2, V_3, \ldots, V_K$.

Throughout this section we will use the following notation unless otherwise stated. $F(x)$ will denote a series of Stieltjes with radius of convergence at least $R > 0$. $\{x_i\}_{i=1}^{\infty}$ will denote a bounded monotone increasing sequence of points, $x_i \in (-R, \infty)$ $(i = 1, 2, \cdots)$ convergent to some point $x^* < \infty$. That is, $-R < x_1 < x_2 < \cdots < x^* < \infty$ and $\lim x_i = x^*$ as $i \to \infty$. The multipoint approximant $f_{P(P)}(x)$ to $F(x)$ which uses information at the first P points, $x_1 < x_2 < \cdots < x_P$, will be denoted by $f_P(x)$. In rational form (cf. Sec. 2) $f_P(x) = A_P(x)/B_P(x)$ where $A_P(x), B_P(x)$ are polynomials of degrees $[(P-1)/2], [P/2]$, respectively.

Lemma 1: $f_P(x)$ can be written uniquely in the form

$$f_P(x) = V_0^P + \sum_{n+1}^{[P/2]} \frac{V_n^P}{(\mathcal{E}_n^P + x)},$$

where $V_0^P = 0$ if P is even, $0 \leq V_0^P < \infty$ if P is odd, $0 < V_n^P < \infty$ $(n = 1, 2, \ldots, [P/2])$, and $R \leq \mathcal{E}_1^P < \mathcal{E}_2^P < \cdots < \mathcal{E}_{[P/2]}^P < \infty$.

Proof: Since $f_P(x)$ may be considered as an extremal case of a series of Stieltjes with radius of convergence at least R [recall Sec. 3 circa Eq. (5)] and since $f_P(x) = A_P(x)/B_P(x)$ as above, it follows that we must be able to write uniquely

$$f_P(x) = V_0^P + \sum_{n=1}^{J} \frac{V_n^P}{(\mathcal{E}_n^P + x)},$$

where $J \leq [P/2]$, $0 \leq V_0^P < \infty$, $0 < V_n^P < \infty$ $(n = 1, 2, \ldots, J)$ and $R \leq \mathcal{E}_1^P < \mathcal{E}_2^P < \cdots < \mathcal{E}_J^P < \infty$. Thus, we need only show that $J = [P/2]$. This is achieved if we show that $A_P(x)$ and $B_P(x)$ possess no common factors. The latter is assured by the uniqueness of the representation of $A_P(x)/B_P(x)$ as the continued fraction obtained by setting $F_P(x) \equiv 0$ in the right-hand side of Eq. (3) wherein we know that none of $a_1, a_2, \ldots, a_P$ vanish. This completes the proof.

Now let $1 \leq M < P$ and let $D(x)$ denote the function

$$D(x) = f_P(x) - f_M(x).$$

Here we shall understand that if $D(x)$ possesses any removeable singularities then these shall be removed. That is, if both $f_P(x)$ and $f_M(x)$ possess a pole of strength V located at $X = -E$, then we define $D(-E) = \lim D(x)$ as $x \to -E$. We will suppose that the poles of $D(x)$ are located at $x = -E_i$ $(i = 1, 2, \ldots, L \leq [M/2] + [P/2])$ where $R \leq E_1 < E_2 < \cdots < E_L < \infty$.

It is easily seen that we can write

$$D(x) = [A_P(x)B_M(x) - A_M(x)B_P(x)]/B_P(x)B_M(x), \tag{10}$$

where any common factors between the numerator and denominator are to be removed. Before any such cancellation is made, it is readily seen that the degree of the numerator in (10) is at most

$$\max\left\{\left[\frac{P-1}{2}\right] + \left[\frac{M}{2}\right]; \left[\frac{M-1}{2}\right] + \left[\frac{P}{2}\right]\right\} = M + \left[\frac{P-M-1}{2}\right].$$

Since $D(x_i) = 0$ $(i = 1, 2, \ldots, M)$, the numerator in (10) must possess the factor

$$(x_1 - x)(x_2 - x)\cdots(x_M - x)$$

which is of degree M. Hence we can write (10) as

$$D(x) = \frac{(x_1 - x)(x_2 - x)\cdots(x_M - x)}{(x + \mathcal{E}_1^P)(x + \mathcal{E}_2^P)\cdots(x + \mathcal{E}_{[P/2]}^P)} \times \frac{R([(P-M-1)/2]; x)}{(x + \mathcal{E}_1^M)(x + \mathcal{E}_2^M)\cdots(x + \mathcal{E}_{[M/2]}^M)}, \tag{11}$$

where we have used the decomposition of Lemma 1, and where $R([(P-M-1)/2]; x)$ denotes a polynomial of degree at most $[(P-M-1)/2]$. In particular, the only common factors between the numerator and denominator of (11) can occur between R and the denominator because by Lemma 1 the zeros of the denominator are located in $(-\infty, -R)$ whereas $-R < x_1 < x_2 < \cdots < x_M < \infty$ by the definition of the sequence $\{x_i\}_{i=1}^{\infty}$.

Lemma 2: In the notation of Lemma 1 we must have

$\mathcal{E}_m^P < \mathcal{E}_m^M (m = 1, 2, \ldots, [M/2])$ and $V_1^P < V_1^M$.

Proof: Consider first the case that $P = M + 1$. Then the polynomial R occurring in (11) must reduce to a constant. This constant must be positive because it follows from Sec. 2 that $f_{M+1}(x) - f_M(x) > 0$ for $x \in (-R, x_1)$. In particular, there can be no common factors between the numerator and denominator of (11) in this case, and thus no pole of $f_{M+1}(x)$ can be coincident in location with any pole of $f_M(x)$ since any such coincidence would imply the existence of a common factor. This means that (11) may be used to evaluate the residues of $f_{M+1}(x)$ and $f_M(x)$ at each of their respective poles. Thus, in the notation of Lemma 1,

$$V_j^{M+1} = \operatorname*{Res}_{x \to -\mathcal{E}_j^{M+1}} D(x), \quad j = 1, 2, \ldots, [(M+1)/2] \tag{12}$$

and

$$V_k^M = -\operatorname*{Res}_{x \to -\mathcal{E}_k^M} D(x), \quad k = 1, 2, \ldots, [M/2].$$

But from Lemma 1 we already know that these residues are positive, and hence the locations of the poles of $f_{M+1}(x)$ and $f_M(x)$ must interlace according to

$$\mathcal{E}_1^{M+1} < \mathcal{E}_1^M < \mathcal{E}_2^{M+1} < \cdots < \begin{cases} \mathcal{E}_{[(M+1)/2]}^{M+1} < \mathcal{E}_{[M/2]}^M & \text{if } M \text{ is even} \\ \mathcal{E}_{[M/2]}^M < \mathcal{E}_{[(M+1)/2]}^{M+1} & \text{if } M \text{ is odd} \end{cases} . \tag{13}$$

In particular, using (12), we obtain the expressions

$$V_1^{M+1} = \frac{\{\text{positive const}\}(x_1 + \mathcal{E}_1^{M+1})(x_2 + \mathcal{E}_1^{M+1}) \cdots (x_M + \mathcal{E}_1^{M+1})}{(\mathcal{E}_2^{M+1} - \mathcal{E}_1^{M+1})(\mathcal{E}_3^{M+1} - \mathcal{E}_1^{M+1}) \cdots (\mathcal{E}_{[(M+1)/2]}^{M+1} - \mathcal{E}_1^{M+1})(\mathcal{E}_1^M - \mathcal{E}_1^{M+1})(\mathcal{E}_2^M - \mathcal{E}_1^{M+1}) \cdots (\mathcal{E}_{[M/2]}^M - \mathcal{E}_1^{M+1})}$$

and

$$V_1^M = \frac{\{\text{positive const}\}(x_1 + \mathcal{E}_1^M)(x_2 + \mathcal{E}_1^M) \cdots (x_M + \mathcal{E}_1^M)}{(\mathcal{E}_1^M - \mathcal{E}_1^{M+1})(\mathcal{E}_2^{M+1} - \mathcal{E}_1^M)(\mathcal{E}_3^{M+1} - \mathcal{E}_1^M) \cdots (\mathcal{E}_{[(M+1)/2]}^{M+1} - \mathcal{E}_1^M)(\mathcal{E}_2^M - \mathcal{E}_1^M)(\mathcal{E}_3^M - \mathcal{E}_1^M) \cdots (\mathcal{E}_{[M/2]}^M - \mathcal{E}_1^M)}$$

from which, by using the inequalities (13), we derive

$$V_1^M > V_1^{M+1}. \tag{14}$$

Since the relations (13) and (14) are true for arbitrary $M = 1, 2, \ldots, P-1$ we can now write down their generalizations. Namely, for $P > M$ we must have

$$\mathcal{E}_1^M > \mathcal{E}_1^P, \mathcal{E}_2^M > \mathcal{E}_2^P, \ldots, \mathcal{E}_{[M/2]}^M > \mathcal{E}_{[M/2]}^P,$$

and $V_1^M > V_1^P$. This completes the proof of the lemma.

We now consider further the function $D(x)$ in the general case $P > M \geq 1$. We define C to be the degree of the highest common factor between $R((P - M - 1)/2]; x)$ and the denominator in Eq. (11). Then it is easily seen that $D(x)$ can have at most

$$[(P - M - 1)/2] - C \geq 0 \tag{15}$$

zeros in the interval $(-\infty, -R)$. Here, and throughout the remainder of this section we count zeros according to their multiplicities.

Now let J denote the number of poles of $f_M(x)$ which have coincident locations with poles of $f_P(x)$. Of these let J_0 be the number of poles at each of which the residue of $D(x)$ vanishes. Then it is easily seen that

$$C = J_0 + J. \tag{16}$$

Further, let J_+ and J_- denote the number of the coincident poles at each of which the residue of $D(x)$ is strictly positive and strictly negative, respectively. Then

$$J = J_0 + J_+ + J_-.$$

Hence, according to our counting, $D(x)$ possesses exactly

$$L = [P/2] + [M/2] - 2J_0 - J_+ - J_-$$

poles located at distinct points in $(-\infty, -R]$. Of these poles, exactly

$$[P/2] - J + J_+$$

have strictly positive residues, and

$$[M/2] - J + J_-$$

have strictly negative residues. We note that

$$[P/2] - J + J_+ \geq 1$$

since we know that $D(x)$ possesses at least one pole with a strictly positive residue, namely the one at $x = -\mathcal{E}_1^P = -E_1$.

Let $x = -E_i^+ (i = 1, 2, \ldots, [P/2] - J + J_+)$, where $R \leq \mathcal{E}_1^P = E_1^+ < E_2^+ < \cdots < E_{[P/2]-J+J_+}^+ < \infty$, denote the locations of the strictly positive poles of $D(x)$. Then we define the intervals $(-E_{j+1}^+, -E_j^+)(j = 1, 2, \ldots, [P/2] - J + J_+ - 1)$ to be *the positive intervals of* $D(x)$. We understand that if $[P/2] - J + J_+ - 1 = 0$, then $D(x)$ possesses no positive intervals.

Lemma 3: $D(x)$ possesses at least one zero on each of its positive intervals which does not contain a pole with strictly negative residue.

Proof: This result follows immediately from the intermediate value theorem for continuous functions. If $D(x)$ does not possess a strictly negative pole in $(-E_{j+1}^+, -E_j^+)$ say, then $D(x)$ is continuous over this interval. Since $D(x) \to -\infty$ as $x \to -E_j^+$ from the left and $D(x) \to +\infty$ as $x \to -E_{j+1}^+$ from the right, the result follows at once.

Lemma 4: Let everything be as defined above. Then $J_0 = J_+ = 0$. In particular, if $\mathcal{E}_r^M = \mathcal{E}_S^P$ for some r, and S, then $V_r^M > V_S^P$.

Proof: The number of positive intervals is

$$[P/2] - J + J_+ - 1$$

Hence, *at most* $\min\{[P/2] - J + J_+ - 1, [M/2] - J + J_-\}$

of the positive intervals can contain a strictly negative pole, and we can assert by Lemma 3 that the number

$$([P/2]-J+J_+-1)-([M/2]-J+J_-)$$
$$=[P/2]-[M/2]-1+J_+-J_-$$

is a rigorous (though, possibly, attainable) lower bound to the number of zeros of $D(x)$ in $(-\infty,-R)$. But from (15) and (16) we have the upper bound

$$[(P-M-1)/2]-J-J_0$$

on the number of zeros of $D(x)$ in $(-\infty,-R)$. Hence, we must have

$$[P/2]-[M/2]-1+J_+-J_-\leq[(P-M-1)/2]-J-J_0$$

or

$$[P/2]-[M/2]-[(P-M-1)/2]-1\leq-2(J_++J_0). \tag{17}$$

If P and M are both even, if P is even and M is odd, or if P and M are both odd, then (17) implies

$$0\leq-2(J_++J_0)$$

which is only possible if $J_+=J_0=0$ since both $J_+,J_0\geq 0$.

If P is odd and M is even, then (17) implies

$$-1\leq-2(J_++J_0),$$

so that again we must have $J_+=J_0=0$.

In particular, if a pole of $f_M(x)$ is coincident in location with a pole of $f_P(x)$, then $D(x)$ must possess a pole with strictly negative strength at this location; whence if $\mathcal{E}_r^M=\mathcal{E}_S^P$ for some r and S then $V_r^M>V_S^P$. This completes the proof.

We see now that $D(x)$ possesses

$$[P/2]-J_-\geq 1$$

distinct positive poles,

$$[P/2]-J_--1\geq 0$$

positive intervals,

$$[M/2]$$

distinct negative poles, and that $D(x)$ can have at most

$$[(P-M-1)/2]-J_-\geq 0$$

zeros in $(-\infty,-R)$.

Lemma 5: No positive interval of $D(x)$ can contain more than one negative pole.

Proof: The lemma is trivially true if

$$[P/2]-J_--1=0$$

or if

$$[M/2]\leq 1.$$

So suppose

$$[P/2]-J_--1>0,\qquad [M/2]>1,$$

and that at least one positive interval contains at least two negative poles. Then on any such positive interval $D(x)$ possesses at least one zero, by an argument similar to that used in Lemma 3.

Furthermore, at most $[M/2]-1$ of the remaining $[P/2]-J_--2$ positive intervals can each contain at least one negative pole. Hence, by an argument similar to that used in Lemma 4, the number

$$([P/2]-J_--2)-([M/2]-2)+1$$
$$=[P/2]-[M/2]+1-J_-$$

is a rigorous lower bound to the number of zeros of $D(x)$ in $(-\infty,-R)$. But $D(x)$ possesses at most

$$[(P-M-1)/2]-J_-$$

zeros in $(-\infty,-R)$. Hence

$$[P/2]-[M/2]+1\leq[(P-M-1)/2]$$

which is impossible. This completes the proof of the lemma by contradiction.

Lemma 6: At most one negative pole of $D(x)$ does not lie in any positive interval.

Proof: We first note that any negative pole of $D(x)$ which is not located in any positive interval of $D(x)$, must be located in $(-\infty,-E^+_{[P/2]-J_-})$ since it follows from Lemma 2 that all negative poles of $D(x)$ must be located in $(-\infty,-E_1)$.

The lemma follows immediately if

$$[M/2]\leq 1,$$

so we suppose

$$[M/2]>1$$

and that at least two negative poles are located in $(-\infty,-E^+_{[P/2]-J_-})$. Then $D(x)$ possesses at least one zero in $(-\infty,-E^+_{[P/2]-J_-})$ by an argument similar to that used in Lemma 3. There are $[P/2]-J_--1$ positive intervals and there remain at most $[M/2]-2$ negative poles with which these intervals might be occupied. Hence, by an argument similar to that used in Lemma 4, we can assert that the number

$$([P/2]-J_--1)-([M/2]-2)+1$$
$$=[P/2]-[M/2]+2-J_-$$

is a rigorous lower bound on the number of zeros of $D(x)$ located in $(-\infty,-R)$. But $D(x)$ possesses at most $[(P-M-1)/2]-J_-$ zeros in $(-\infty,-R)$. Hence

$$[P/2]-[M/2]+2\leq[(P-M-1)/2]$$

which is impossible. This completes the proof of the lemma by contradiction.

Lemma 7: Let $x=-E_i\,(i=1,2,\ldots,L=[P/2]+[M/2]-J_-)$ where $R\leq\mathcal{E}_1^P=E_1<E_2<\cdots<E_L<\infty$ denote the locations of the poles of $D(x)$ as before. Then if $x=-E_j$ for some $j\in\{2,3,\ldots,L-1\}$ corresponds to a pole of $D(x)$ with negative residue then the poles of $D(x)$ located at both $x=-E_{j+1}$ and $x=-E_{j-1}$ have positive residues; and $D(x)>0$ for $x\in(-E_{j+1},-E_j)$,

$D(x) < 0$ for $x \in (-E_j, -E_{j-1})$. If $D(x)$ possesses a pole with negative residue located at $x = -E_L$ then the pole located at $x = -E_{L-1}$ has a positive residue and $D(x) < 0$ for $x \in (-E_L, -E_{L-1})$.

Proof: The statements that if $D(x)$ has a negative residue at $x = -E_j$ then $D(x)$ has a positive residue at $x = -E_{j-1}$, and at $x = -E_{j+1}$, if $j < L$, follow immediately from Lemmas 5 and 6.

That $D(x) > 0$ for $x \in (-E_{j+1}, -E_j)$ and $D(x) < 0$ for $x \in (-E_j, -E_{j-1})$ if $x = -E_j$ corresponds to a pole with negative residue when $j < L$, now follows at once if we prove that $D(x)$ possesses no zeros on any positive interval which contains a pole with negative residue. To prove this we assume the converse: Suppose $D(x)$ vanishes on some positive interval which contains a negative pole. Then it is easily seen by applying the intermediate value theorem that $D(x)$ must possess at least *two* zeros on any such positive interval. A lower bound to the number of zeros of $D(x)$ in $(-\infty, -R)$ is then

$$([P/2] - J_- - 2) - ([M/2] - 1) + 2 = [P/2] - [M/2] + 1 - J_-$$

which as in earlier lemmas we conclude is not possible.

Similarly we can prove that if $D(x)$ possesses a pole with negative residue at $x = -E_L$ then $D(x) < 0$ for $x \in (-E_L, -E_{L-1})$. The proof of the lemma is thus completed.

We will need one more result.

Lemma 8: Let D_R denote any closed bounded domain interior to the cut $(-\infty \leq z \leq -R)$ complex plane. Then the sequence of approximants $\{f_P(z)\}_{P=1}^{\infty}$ converges uniformly to $f(z)$ for $z \in D_R$.

Proof: We may suppose without loss of generality that $x_n \in D_R (n = 1, 2, \ldots, \infty)$.

Then it is shown in GB that $\{f_P(z)\}_{P=1}^{\infty}$ converges to *some* series of Stieltjes $\tilde{F}(z)$ with radius of convergence at least R, for all $z \in D_R$. Thus, both $\tilde{F}(z)$ and $F(z)$ are analytic with no singularities for $z \in D_R$, whence so is $B(z) = \tilde{F}(z) - F(z)$. Since $\tilde{F}(x_n) = \lim f_P(x_n) = F(x_n)$ as $P \to \infty$, it follows that $B(x_n) = 0 (n = 1, 2, \ldots, \infty)$. Thus $B(z)$ vanishes on a limit point sequence in D_R, and so it vanishes identically[17] throughout D_R. Hence $f_P(z)$ converges to $F(z)$ for all $z \in D_R$, and the convergence is uniform since D_R is compact. This completes the proof.

Theorem: Let $G(x)$ be a series of Stieltjes of the special form (9). Let $g_P(x)$ denote the multipoint Padé approximant to $G(x)$ which uses the P pieces of information $\{G(x_i)\}_{i=1}^{P}$ where $-R < x_1 < x_2 < \cdots < x_P < \infty$. Let the expansion of $g_P(x)$ be denoted as in Lemma 1, $f_P(x)$ being replaced by $g_P(x)$. Then $\mathcal{E}_j < \mathcal{E}_j^P (j = 1, 2, \ldots, \min\{[P/2], K\})$ and $V_1 < V_1^P$. If $\mathcal{E}_r = \mathcal{E}_S^P$ for some r and S then $V_r < V_S^P$.

Furthermore, let $D^*(x)$ denote the function

$$D^*(x) = G(x) - g_P(x), \qquad x \in (-R', -R],$$

and let $x = -E_i (i = 1, 2, 3, \ldots, L^* \leq [P/2] + K)$ denote the locations of the poles of $D^*(x)$ which lie in $(-R', -R]$, where $\mathcal{E}_1 = E_1 < E_2 < \cdots < E_{L^*} < R'$. If, for some $l \in \{2, 3, \ldots, L^* - 1\}$, $D^*(x)$ has a pole with a negative residue located at $x = -E_l$, then the poles located at $x = -E_{l+1}$ and $x = -E_{l-1}$ have positive residues, and $D^*(x) \geq 0$ for $x \in (-E_{l+1}, -E_l)$, $D^*(x) \leq 0$ for $x \in (-E_l, -E_{l-1})$. If $x = -E_{L^*}$ is the location of a pole of $D^*(x)$ with a negative residue then $x = -E_{L^*-1}$ corresponds to a pole with a positive residue, and $D^*(x) \leq 0$ for $x \in (-E_{L^*}, -E_{L^*-1})$.

Proof: First extend the set of points $x_1 < x_2 < \cdots < x_P$ to a sequence of points $\{x_i\}_{i=1}^{\infty}$ as defined at the beginning of this section.

Let $Q \geq P$ be a finite integer and let $h_Q(x)$ denote the $Q(Q)$ approximant to $H(x)$ which uses the Q pieces of information $\{H(x_q): q = 1, 2, \ldots, Q\}$.

Now let

$$g_{(2K+Q)}(x) = \sum_{k=1}^{K} V_k/(\mathcal{E}_k + x) + h_Q(x). \tag{18}$$

We note that: (i) $g_{(2K+Q)}(x_i) = g_P(x_i)$ $(i = 1, 2, \ldots, P)$.

(ii) The poles of $g_{(2K+Q)}(x)$ which lie in $(-R', -R]$ are those represented by the sum on the right-hand side of (18), their strengths and locations being independent of Q, since by Lemma 1 the poles of $h_Q(x)$ are located in $(-\infty, -R')$.

(iii) If $D_{R'}$ denotes any closed bounded domain, interior to the cut $(-\infty \leq z \leq -R')$ complex plane, and if $D'_{R'}$ denotes the same domain with the points $x = -\mathcal{E}_k$ $(k = 1, 2, \ldots, K)$ removed, then $\{g_{(2K+Q)}(z)\}_{Q=P}^{\infty}$ converges uniformly to $G(z)$ for $z \in D'_{R'}$, since by Lemma 8 $\{h_Q(z)\}_{Q=P}^{\infty}$ converges uniformly to $H(z)$ for $z \in D_{R'}$.

Now it is easily shown that for fixed Q there exists a series of Stieltjes $G^Q(x)$, with radius of convergence R^Q satisfying $-R < -R^Q < x_1$, such that $g_{(2K+Q)}(x)$ is the $(2K+Q)(2K+Q)$ approximant to $G^Q(x)$ with $G^Q(x_j) = g_{(2K+Q)}(x_j)(j = 1, 2, \ldots, 2K+Q)$. But then by (i) $g_P(x_i) = G^Q(x_i)(i = 1, 2, \ldots, P)$ and so $g_P(x)$ is a $P(P)$ approximant to $G^Q(x)$. Thus, in the obvious notation, we can denote

$$g_P(x) = g_P^Q(x) \quad \text{and} \quad g_{(2K+Q)}(x) = g^Q_{(2K+Q)}(x)$$

In particular, Lemmas 2, 4, and 7 apply, pertaining now to the relationship between $g_P^Q(x)$ and $g^Q_{(2K+Q)}(x)$ rather than $f_M(x)$ and $f_P(x)$, respectively, and pertaining now to the difference

$$D^Q(x) = g^Q_{(2K+Q)}(x) - g_P^Q(x)$$

rather than to $D(x) = f_P(x) - f_M(x)$.

The poles of $g_P^Q(x) = g_P(x)$ are, in the notation of Lemma 1, represented by

$$g_P(x) = V_0^P + \sum_{n=1}^{[P/2]} \frac{V_n^P}{(\mathcal{E}_n^P + x)}$$

and hence, recalling (ii), we have by Lemma 2 that $\mathcal{E}_k^P > \mathcal{E}_k (k = 1, 2, \ldots, \min\{[P/2], K\})$ and $V_1^P > V_1$.

Similarily, by Lemma 4 we have that if $\mathcal{E}_r^P = \mathcal{E}_S$ for some $r \in \{1, 2, \ldots, [P/2]\}$ and $S \in \{2, 3, \ldots, K\}$ then $V_r^P > V_S$.

The remainder of the theorem follows from Lemma 7. To see this we need only note that the poles of

$$D^Q(x) = g^Q_{(2K+Q)}(x) - g_P^Q(x)$$

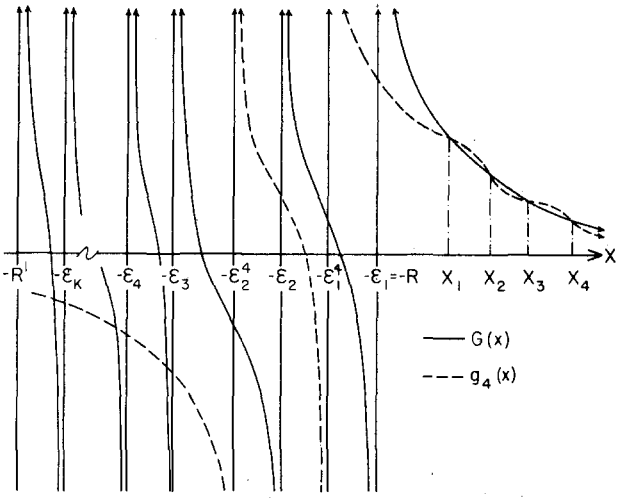

FIG. 4. Sketch illustrating the bounding relationship between a series of Stieltjes $G(x)$, of the special form (9), and a 4(4) multipoint Padé approximant to it, $g_4(x)[=g_{4(4)}(x)]$. The given information is $G(x_i)$ $(i=1,2,3,4)$ where $-R<x_1<x_2<x_3<x_4<\infty$. Here we have supposed that $\mathcal{E}_1<\mathcal{E}_1^4<\mathcal{E}_2<\mathcal{E}_2^4<\mathcal{E}_3<\cdots<\mathcal{E}_K$ (see text for notation).

which lie in $(-R', -R]$ are precisely those of $D^*(x)$ which lie in $(-R', -R]$; and that $\{D^Q(x)\}_{Q=P}^{\infty}$ converges uniformly to $D^*(x)$ for $x\in(-E_{L^*}, -E_{L^*-1})\cup(-E_{L^*-1}, -E_{L^*-2})\cup\cdots\cup(-E_2, -E_1)$ since $g_P^Q(x)=g_P(x)$, and by (iii) $g_{(2K+Q)}^Q(x)=g_{(2K+Q)}(x)$ converges uniformly to $G(x)$ over this range.

This completes the proof of the theorem.

Example: Suppose that $G(x)$ has the special form (9), and that we are given four pieces of information about $G(x)$: $G(x_i)$ $(i=1,2,3,4)$ with $-R<x_1<x_2<x_3<x_4<\infty$. Then the multipoint Padé approximant $g_4(x)$ which corresponds to this set of information can be written in the form

$$g_4(x)=\frac{V_1^4}{(\mathcal{E}_1^4+x)}+\frac{V_2^4}{(\mathcal{E}_2^4+x)}$$

The theorem tells us that a possible relationship between the $\mathcal{E}_k$ $(k=1,2,\ldots,K)$ and the $\mathcal{E}_i^4$ $(i=1,2)$ might be

$$\mathcal{E}_1<\mathcal{E}_1^4<\mathcal{E}_2<\mathcal{E}_2^4<\mathcal{E}_3<\mathcal{E}_4<\cdots<\mathcal{E}_k.$$

In this case the bounding relationship between $g_4(x)$ and $G(x)$ would be as illustrated in Fig. 4. Here we have that $g_4(x)\leqslant G(x)$ for $x\in(-\mathcal{E}_3, -\mathcal{E}_2^4)\cup(-\mathcal{E}_2, -\mathcal{E}_1^4)\cup(-\mathcal{E}_1, x_1)\cup(x_2, x_3)\cup(x_4, \infty)$, and $g_4(x)\geqslant G(x)$ for $x\in(-\mathcal{E}_2^4, -\mathcal{E}_2)\cup(-\mathcal{E}_1^4, -\mathcal{E}_1)\cup(x_1, x_2)\cup(x_3, x_4)$.

Other possible relations between the $\mathcal{E}_k$ and the $\mathcal{E}_i^4$ could be

$$\mathcal{E}_1<\mathcal{E}_2<\mathcal{E}_1^4<\mathcal{E}_3<\mathcal{E}_4<\mathcal{E}_2^4<\mathcal{E}_5<\cdots<\mathcal{E}_K$$

and

$$\mathcal{E}_1<\mathcal{E}_1^4<\mathcal{E}_2<\mathcal{E}_3=\mathcal{E}_2^4<\mathcal{E}_4<\mathcal{E}_5<\cdots<\mathcal{E}_K$$

for example, but one could not have

$$\mathcal{E}_1<\mathcal{E}_2<\mathcal{E}_1^4<\mathcal{E}_2^4<\mathcal{E}_3<\mathcal{E}_4<\cdots<\mathcal{E}_K \quad \text{say.}$$

In each case the theorem further tells us that $V_1<V_1^4$, and in the case where $\mathcal{E}_3=\mathcal{E}_2^4$ we must have $V_3<V_2^4$.

The above theorem can easily be extended to a general $N(P)$ approximant to $G(x)$. This is achieved by allowing various subsets of the interpolation points $x_1<x_2<\cdots<x_P$ to tend to coincidence, as was done near the end of Sec. 2. If this approach is used then several of the statements in the theorem must be weakened slightly. For example, we are forced to conclude that $\mathcal{E}_j^P\geqslant\mathcal{E}_j$ rather than $\mathcal{E}_j^P>\mathcal{E}_j$ $(j=1,2,\ldots,\min\{[P/2],K\})$ and so on.

However, Lemmas 1–8 *can* be rederived in the more general context of a sequence of $N(P)$ approximants, and it is possible to establish that the statements of the theorem are *strictly* true in the general case. In particular, they apply to the usual $[n,n]$ and $[n,n-1]$ one-point Padé approximants. Furthermore, it is possible to strengthen various statements in the theorem as it stands: Such a statement as "$D^*(x)\geqslant 0$ for $x\in(-E_{l+1}, -E_l)$" can be replaced by "$D^*(x)>0$ for $x\in(-E_{l+1}, -E_l)$," and so on, by considering the relationship between two successive approximants $g_P(x), g_{P+1}(x)$ to $G(x)$. Such formal generalization and strengthening of the theorem has not been set down here since the details involved tend to confuse what is basically a simple idea, and since in all applications it makes no difference if we say $>$ or $\geqslant$.

The bounding properties stated in the theorem are all "best possible," but with a qualification. To see the best possible nature of the results we only need to consider the case where $G(x)$ is an *extremal* case of a series of Stieltjes: We can take $G(x)$ to be

$$G^{\mathcal{E}}(x)=\sum_{k=1}^{K}\frac{V_k}{(\mathcal{E}_k+x)}$$

and then construct any $2K(P)$ approximant to $G^{\mathcal{E}}(x)$. The approximant will of course be $G^{\mathcal{E}}(x)$ itself. Although $G^{\mathcal{E}}(x)$ is not strictly a series of Stieltjes, because the corresponding distribution function has only a *finite* number of points of increase, there exist infinitely many true series of Stieltjes which agree with $G^{\mathcal{E}}(x)$ on the information set, and which lie arbitrarily close to it on any interval of interest. Thus, in the theorem, we cannot know *on the basis of the given information* that the approximant $g_P(x)$ does not in fact lie arbitrarily close to $G(x)$ on any interval of interest. Hence, the bounding properties of $g_P(x)$ [in general, of $g_{N(P)}(x)$] with respect to $G(x)$ must be best possible. In particular the $\mathcal{E}_j^P$ supply the best possible upper bounds to the $\mathcal{E}_k$, and V_1^P is a best possible upper bound to V_1. However, we must treat the functional bounding properties of $g_P(x)$ with respect to $G(x)$ with some care. For example, we cannot assert that $g_P(x)$ imposes an upper bound on $G(x)$ for $x\in(-\mathcal{E}_1^P, -\mathcal{E}_1)$ without first knowing that $-\mathcal{E}_2<-\mathcal{E}_1^P<-\mathcal{E}_1$ and, in particular, without specifically knowing the values of $\mathcal{E}_1$ and $\mathcal{E}_2$. But such knowledge constitutes additional information which has not been used in the construction of the approximant. Hence we cannot precisely assert that such bounds are best possible on the basis of the given information. If we had not known $\mathcal{E}_1$ and $\mathcal{E}_2$ then we could only say "$g_P(x)$ imposes a best possible upper bound on $G(x)$ for x lying in some (unspecified) open interval located directly to the right of $-\mathcal{E}_1^P$," for example. In the next section we will see how a specific knowledge of $\mathcal{E}_1$ and $\mathcal{E}_2$, say, can be incorporated into the approximant and yields bounds on $G(x)$ which will indeed usually be best possible for $-\mathcal{E}_2<x<-\mathcal{E}_1$, say.

Despite the above qualification, the multipoint Padé

approximant may often provide a simple method for imposing bounds to a series of Stieltjes in the region of poles. Such an application relates to the dynamical polarizability, described in the introduction. Here one usually has a fair idea of the first few "excitation energies" (the $\mathcal{E}_k$) for the system under consideration; but these are not used in constructing the usual $[n, n-1]$ and $[n, n]$ one-point Padé approximants to the polarizability. As stated above, the present theory applies to these approximants, and, thus, it is possible to impose bounds on the dynamical polarizability at frequencies equivalent to energies *higher* than the first excitation energy of the system. Such a bounding procedure has not been applied, but it has been claimed (Ref. 18, near bottom p. 47), in such cases that in addition to $V_1^P > V_1$, one also has $V_2^P > V_2$, $V_3^P > V_3$, and so on. That the latter statements cannot, in general, be true can be seen by constructing the usual [2, 1] Padé approximant to the extremal series of Stieltjes

$$G^{\mathcal{E}}(x) = \frac{(1/1.98)}{(1+x)} + \frac{(1\,600)}{(2+x)} + \frac{(90/2.2)}{(3+x)}.$$

One obtains the approximant

$$g_{4(1)}(x) = [2,1] = \frac{(1\,303.21/1.98)}{(1.9+x)} + \frac{(1\,944.81/1.98)}{(2.1+x)}$$

for which one has $V_1^4 = (1\,303.21/1.98) > (1/1.98) = V_1$, but $V_2^4 = (1\,944.81/1.98) < 1\,600 = V_2$. We note that the other assertions in the theorem can easily be verified for this example. In particular, it is an immediate consequence of the theorem that the $\mathcal{E}_j^P$ give not only upper bounds to the $\mathcal{E}_k$ but also they supply *lower* bounds in the following way: Between any successive pair of the $\mathcal{E}_j^P$ lying in $(-R', -R]$ there must exist at least one pole of the original series of Stieltjes $G(x)$. Thus, in this example, we have not only $\mathcal{E}_1 = 1 < 1.9 = \mathcal{E}_1^4$ and $\mathcal{E}_2 = 2 < 2.1 = \mathcal{E}_2^4$, but also we are assured *a priori* that $G^{\mathcal{E}}(x)$ has a pole located in the interval $[-2.1, -1.9]$. Recalling our earlier remarks about extremal series of Stieltjes it is easily seen that there is no loss of generality in using such a function in this example.

The correct statement of the relationship between the V_k and the V_j^P is almost certainly an extension of the "Cumulative Distribution" theorem which occurs in moment theory.[19]

We now consider the analog of the above theorem for the complementary multipoint Padé approximant. Let $G(x)$ be as in (9), and let $g_P^C(x)$ $[= g_{P(P)}^C(x)]$ denote the complementary multipoint Padé approximant which uses the P pieces of information $\{G(x_i)\}_{i=1}^P$, where $-\mathcal{E}_1^L < x_1 < x_2 < \cdots < x_P < \infty$, together with the lower bound $\mathcal{E}_1^L \leq \mathcal{E}_1$ for the radius of convergence of $G(x)$. We suppose that $\mathcal{E}_1^L < \mathcal{E}_1$ since the case $\mathcal{E}_1^L = \mathcal{E}_1$ is treated in the next section. Then we note that $g_P^C(x)$ can be constructed in the following manner.

If we let

$$\begin{aligned} G_1(x) &= \frac{(x+\mathcal{E}_1^L)G(x) - (x_1+\mathcal{E}_1^L)G(x_1)}{(x-x_1)} \\ &= \sum_{k=1}^{K} \frac{(\mathcal{E}_k - \mathcal{E}_1^L)V_k}{(\mathcal{E}_k + x_1)(\mathcal{E}_k + x)} \\ &\quad + \frac{(x+\mathcal{E}_1^L)H(x) - (x_1+\mathcal{E}_1^L)H(x_1)}{(x-x_1)} \\ &= \sum_{k=1}^{K} \frac{V_k^{(1)}}{(\mathcal{E}_k + x)} + H_1(x) \end{aligned} \tag{19}$$

in the obvious notation, then it is easy to see that the $V_k^{(1)}$ are positive and $H_1(x)$ is a series of Stieltjes with radius of convergence at least R'. Hence $G_1(x)$ is itself a series of Stieltjes of the same form as $G(x)$, the only difference being that the strengths of the poles are decreased. Now, we can use (19) to transform the original P pieces of information $\{G(x_i)\}_{i=1}^P$ into a set of $(P-1)$ pieces of information, $\{G_1(x_j)\}_{j=2}^P$, about $G_1(x)$. [We cannot determine $G_1(x_1) = G(x_1) + (x_1 + \mathcal{E}_1^L)G^{(1)}(x_1)$ since this value depends on $G^{(1)}(x_1)$.] Hence we can form the $(P-1)(P-1)$ multipoint Padé approximant to $G_1(x)$, which we will denote simply by $g_{(P-1)}(x)$, which corresponds to the transformed set of information and thus satisfies

$$g_{(P-1)}(x_j) = G_1(x_j), \qquad j = 2, 3, \ldots, P.$$

If we rewrite (19) as

$$G(x) = [(x-x_1)G_1(x) + (x_1 + \mathcal{E}_1^L)G(x_1)]/(x + \mathcal{E}_1^L) \tag{20}$$

and then replace $G_1(x)$ by $g_{(P-1)}(x)$, it is easy to show that we obtain the desired approximant. That is,

$$g_P^C(x) = [(x-x_1)g_{(P-1)}(x) + (x_1 + \mathcal{E}_1^L)G(x_1)]/(x + \mathcal{E}_1^L) \tag{21}$$

To see this we note first that the degrees of the numerator and denominator here are $[P/2]$ and $[(P+1)/2]$, respectively, since the corresponding degrees for $g_{(P-1)}(x)$ are $[(P-2)/2]$ and $[(P-1)/2]$, respectively. Further, the approximant clearly possesses a pole located at $x = -\mathcal{E}_1^L$ and satisfies $g_P^C(x_i) = G(x_i)$ for $i = 1, 2, \ldots, P$. Hence, by uniqueness, we conclude that we have indeed constructed the desired multipoint Padé approximant, as discussed in Sec. 3.

It is now a simple matter to deduce the bounding relationship between $g_P^C(x)$ and $G(x)$. We need only to compare (21) and (20), making use of the previously established bounding properties of $g_{(P-1)}(x)$ with respect to $G_1(x)$. In this manner the bounding properties of $g_P^C(x)$ for $-\mathcal{E}_1^L < x < \infty$, as established in Sec. 3, are reconfirmed. For $-\mathcal{E}_1 < x < -\mathcal{E}_1^L$ we find $g_P^C(x) < G(x)$. For $-R' < x < -\mathcal{E}_1$ we find that the relationship between the two functions is almost exactly the same as given in the theorem for $g_P(x)$ and $G(x)$. If the poles of $g_P^C(x)$ are located at $x = -\mathcal{E}_i^C (i = 1, 2, \ldots, [(P+1)/2])$ with $-\mathcal{E}_{[(P+1)/2]}^C < -\mathcal{E}_{[(P+1)/2]-1}^C < \cdots < -\mathcal{E}_2^C < -\mathcal{E}_1^C = -\mathcal{E}_1^L$, then the role of $\mathcal{E}_j^P$ in the theorem is now played by $\mathcal{E}_{j+1}^C$ $(j = 1, 2, \ldots, [(P-1)/2])$. In particular, we easily find that $\mathcal{E}_j < \mathcal{E}_{j+1}^C (j = 1, 2, \ldots, \min\{K, [(P-1)/2]\})$ and that the bounding relations between $g_P^C(x)$ and $G(x)$ on the intervals between these poles are the same as in the theorem. If $\mathcal{E}_r = \mathcal{E}_S^C$ for some admissable r and S then $V_r < V_S^C$, where $V_i^C > 0$ denotes the strength of the pole of $g_P^C(x)$ at $x = -\mathcal{E}_i^C$. Moreover, if $\mathcal{E}_1 = \mathcal{E}_1^L$ then $V_1 < V_1^C$, as is shown in the next section. However, in general, there are apparently no other simple bounding relationships between the strengths of the poles of $g_P^C(x)$ and those of $G(x)$.

The bounding properties described here must be best possible, on the basis of the given information, with the same sort of qualification as followed the theorem. This result follows immediately from the best possible nature of the bounding properties of $g_{(P-1)}(x)$ with respect to $G_1(x)$.

These results can be rigorously generalized so that they apply for $N \geq P$. For example, if one assumes that the

theorem itself is true in this case then one can use an $(N-1)(P)$ or $(N-1)(P-1)$ approximant to $G_1(x)$ in place of $g_{(P-1)}(x)$ in the above derivation. However, it is simpler to follow the limiting argument given at the end of Secs.2 and 3. In this way one sees how the bounding properties of $g^C_{N(P)}(x)$ in the region of poles are determined by those of $g^C_{N(N)}(x)$.

We note that the relationship between the two approximants $g_{N(P)}(x)$ and $g^C_{N(P)}(x)$, themselves, is immediate from the theorem when one observes that $g_{N(P)}(x)$ is not only an $N(P)$ approximant to $G(x)$, but also to $g^C_{N(P)}(x)$, itself an extremal series of Stieltjes.

6. FIXING THE LOCATIONS OF THE POLES

We suppose here that $G(x)$ is a series of Stieltjes of the form (9) and that, in addition to the usual N pieces of information at P points, we also know the locations of the first L discrete poles $x = -\mathcal{E}_k\,(k = 1, 2, \ldots, L \leq K)$. Without loss of generality we will assume $L = K$ and that we know R' (a lower bound to), the radius of convergence of $H(x)$. Then, providing $N > K$, it is possible to define a multipoint Padé approximant, denoted $g_{K+N(P)}(x)$, and a complementary approximant, denoted $g^C_{K+N(P)}(x)$, which incorporate the additional information:

$$g_{K+N(P)}(x) = A(x)/B(x), \tag{22}$$

where $A(x)$ and $B(x)$ are *the* polynomials of degrees $[(N+K-1)/2]$ and $[(N+K)/2]$, respectively, which are uniquely specified by the requirements

$$g^{(n)}_{K+N(P)}(x_m) = G^{(n)}(x_m), \quad n = 0, 1, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P$$

together with

$$B(-\mathcal{E}_k) = 0, \quad k = 1, 2, \ldots, K$$

and a normalization condition

$$B(0) = 1.$$

In a similar way,

$$g^C_{K+N(P)}(x) = C(x)/D(x), \tag{23}$$

where $C(x)$ and $D(x)$ are *the* polynomials of degrees $[(N+K)/2]$ and $[(N+K+1)/2]$, respectively, which are uniquely specified by the requirements

$$(g^C_{K+N(P)})^{(n)}(x_m) = G^{(n)}(x_m), \quad n = 0, 1, \ldots, N_m - 1, \quad m = 1, 2, \ldots, P$$

together with

$$D(-R') = 0, \quad D(-\mathcal{E}_k) = 0 \quad k = 1, 2, \ldots, K$$

and a normalization condition

$$D(0) = 1.$$

To establish the existence and bounding properties of these approximants we will follow a method which is closely related to one used by Tang[20] to prove some of the present results in the case of given information at a single point. For notational simplicity we will take $N = P$, and then describe how the results can be generalized. We proceed by making repeated application of (19), except that now we replace $\mathcal{E}_1^L$ successively by the exact values $\mathcal{E}_1, \mathcal{E}_2, \ldots, \mathcal{E}_K$. That is, let

$$G_0(x) = G(x)$$

and

$$G_k(x) = \frac{(x+\mathcal{E}_k)G_{k-1}(x) - (x_k+\mathcal{E}_k)G_{k-1}(x_k)}{(x-x_k)}, \quad k = 1, 2, \ldots, K \tag{24}$$

then

$$G_k(x) = \sum_{r=k+1}^{K} \frac{V_r^{(k)}}{(\mathcal{E}_r + x)} + H_k(x), \tag{25}$$

where

$$V_r^{(k)} = \frac{(\mathcal{E}_r - \mathcal{E}_k)V_r^{(k-1)}}{(\mathcal{E}_r + x_k)} \quad \text{with } V_r^{(0)} = V_r$$

and

$$H_k(x) = \frac{(x+\mathcal{E}_k)H_{k-1}(x) - (x_k+\mathcal{E}_k)H_{k-1}(x_k)}{(x-x_k)} \tag{26}$$

with $H_0(x) = H(x)$. Then, by using (26) it is easy to show that since $H(x)$ is a series of Stieltjes with radius of convergence (at least) R', so is $H_k(x)\,(k = 1, 2, \ldots, K)$. Thus, since the $V_r^{(k)}$'s in (25) are positive, we see that $G_k(x)$ is itself a series of Stieltjes of the same form as $G(x)$, except that the poles located at $x = -\mathcal{E}_1$, $x = -\mathcal{E}_2$, $\ldots, x = -\mathcal{E}_k\,(k = 1, 2, \ldots, K)$, have been removed. In particular,

$$G_K(x) = H_K(x)$$

is simply a series of Stieltjes with radius of convergence (at least) R'.

Now, we can use (24) successively to transform the original set of information $\{G(x_m)\}_{m=1}^P$ into a set of $(P-K)$ pieces of information about $G_K(x)$, namely $\{G_K(x_m)\}_{m=K+1}^P$. This transformed set of information, together with the number R', can now be used to construct the usual complementary pair of multipoint Padé approximants to $G_K(x)$, which we will denote here simply by $g_{P-K}(x)$ and $g^C_{P-K}(x)$.

We now rewrite (24) as

$$G_{K-l}(x) = \frac{(x-x_{K-l+1})G_{K-l+1}(x) + (x_{K-l+1}+\mathcal{E}_{K-l+1})G_{K-l}(x_{K-l+1})}{(x+\mathcal{E}_{K-l+1})}, \quad l = 1, 2, \ldots, K \tag{27}$$

and consider the two sequences of approximants defined by

$$g_{P-K+l}(x) = \frac{(x-x_{K-l+1})g_{P-K+l-1}(x) + (x_{K-l+1}+\mathcal{E}_{K-l+1})G_{K-l}(x_{K-l+1})}{(x+\mathcal{E}_{K-l+1})},$$

$$g^C_{P-K+l}(x) = \frac{(x-x_{K-l+1})g^C_{P-K+l-1}(x) + (x_{K-l+1}+\mathcal{E}_{K-l+1})G_{K-l}(x_{K-l+1})}{(x+\mathcal{E}_{K-l+1})}, \quad l = 1, 2, \ldots, K. \tag{28}$$

[We already know the numbers $G_{K-l}(x_{K-l+1})$ from our original scheme (24)].

We first show that the two approximants corresponding to $l = K$ in (28) are precisely those defined in (22) and (23), in the case $N = P$. Indeed, we have

$$g_{P-K}(x_m) = g^C_{P-K}(x_m) = G_K(x_m), \qquad m = K+1, K+2, \ldots, P,$$

whence from (27) and (28)

$$g_{P-K+1}(x_m) = g^C_{P-K-1}(x_m) = G_{K-1}(x_m), \qquad m = K, K+1, \ldots, P$$

and so on, until we obtain

$$g_P(x_m) = g^C_P(x_m) = G_0(x_m) = G(x_m), \qquad m = 1, 2, \ldots, P.$$

Furthermore, starting with $g_{P-K}(x)$ and $g^C_{P-K}(x)$ in rational form, we find that

$$g_P(x) = \tilde{A}(x)/\tilde{B}(x) \quad \text{and} \quad g^C_P(x) = \tilde{C}(x)/\tilde{D}(x),$$

where $\tilde{A}(x)$ and $\tilde{B}(x)$ are polynomials of degrees $[(P+K-1)/2]$ and $[(P+K)/2]$, respectively; and where $\tilde{C}(x)$ and $\tilde{D}(x)$ are of degrees $[(P+K)/2]$ and $[(P+K+1)/2]$, respectively. Finally, it is clear that $g_P(x)$ has poles located at $x = -\mathcal{E}_k$ $(k = 1, 2, \ldots, K)$ and that $g^C_P(x)$ has, in addition, a pole located at $x = -R'$. Thus, comparing the above statements with (22) and (23), and using the evident uniqueness of these approximants, we conclude that

$$g_P(x) = g_{K+P(P)}(x) \quad \text{and} \quad g^C_P(x) = g^C_{K+P(P)}(x).$$

We note here that we can also obtain a $g_{P+P(P)}(x)$ [which corresponds to the case $K = P$]. To achieve this we use $g_{K-K}(x) = g_0(x) \equiv 0$ as the "starting" approximant in (28). Since, in this case, we have *no* information about $G_K(x)$, $g_0(x)$ is a best possible lower bound for $G_K(x)$. However, we cannot obtain a $g^C_{P+P(P)}(x)$.

The bounding properties of these two approximants are now readily deduced from the already established bounding properties of $g_{P-K}(x)$ and $g^C_{P-K}(x)$ with respect to $G_K(x)$. We simply compare (27) and (28) at each successive step $l = 1, 2, \ldots, K$. For example, we know that $g_{P-K}(x) < G_K(x)$ for $-R' < x < x_{K+1}$, $g_{P-K}(x) > G_K(x)$ for $x_{K+1} < x < x_{K+2}$, and so on; whence it follows immediately that

$$\begin{aligned} g_{P-K+1}(x) &< G_{K-1}(x) \quad \text{for } -R' < x < -\mathcal{E}_K \\ &> G_{K-1}(x) \quad \text{for } -\mathcal{E}_K < x < x_K \\ &< G_{K-1}(x) \quad \text{for } x_K < x < x_{K+1} \\ &> G_{K-1}(x) \quad \text{for } x_{K+1} < x < x_{K+2}, \quad \text{and so on.} \end{aligned}$$

Proceeding in this manner, we finally find that $g_P(x) = g_{K+P(P)}(x) < G_0(x) = G(x)$ for $-R' < x < -\mathcal{E}_1$, and that the direction of the bound is thereafter successively reversed on each of the following successive intervals, $(-\mathcal{E}_K, -\mathcal{E}_{K-1})$, $(-\mathcal{E}_{K-1}, -\mathcal{E}_{K-2}), \ldots, (-\mathcal{E}_1, x_1)$, $(x_1, x_2), \ldots, (x_K, x_{K+1}), \ldots, (x_{P-1}, x_P), (x_P, \infty)$. In a similar fashion we find that the bounding properties of the complementary approximant $g^C_P(x) = g^C_{K+P(P)}(x)$ are, indeed, the precise complement to those given above.

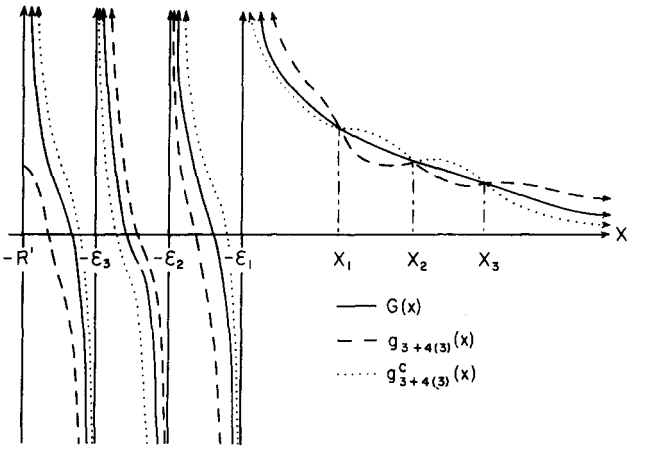

FIG. 5. Sketch illustrating the bounding relationship between a typical $g_{3+4(3)}(x)$, its complement $g^C_{3+4(3)}(x)$, and the series of Stieltjes which they approximate, $G(x) = \sum_{k=1}^{3} V_k/(\mathcal{E}_k + x) + H(x)$. Here the given information used to construct these approximants is: $G(x_1)$, $G(x_2)$, $G^{(1)}(x_2)$, and $G(x_3)$, where $-\mathcal{E}_1 < x_1 < x_2 < x_3 < \infty$; the numbers $\mathcal{E}_1 < \mathcal{E}_2 < \mathcal{E}_3$; and R' (a lower bound to), the radius of convergence of $H(x)$. We have supposed that the pole strengths of the approximants are indeed positive, whence the indicated bounding properties are best possible.

That is, we have

$$\begin{aligned} g^C_{K+P(P)}(x) &> G(x) \quad \text{for } -R' < x < -\mathcal{E}_K \\ &< G(x) \text{ for } -\mathcal{E}_K < x < -\mathcal{E}_{K-1}, \quad \text{and so on.} \end{aligned}$$

From these bounding relations one now readily deduces the bounding properties of the strengths of the "fixed" poles of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$. Let $\tilde{V}_1, \tilde{V}_2, \ldots, \tilde{V}_K$ and $\tilde{V}^C_1, \tilde{V}^C_2, \ldots, \tilde{V}^C_K$ denote the residues of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$, respectively, evaluated at $x = -\mathcal{E}_1, -\mathcal{E}_2, \ldots, -\mathcal{E}_K$, in that order. Then we have $\tilde{V}^C_k < V_k < \tilde{V}_k$ or $\tilde{V}^C > V_k > \tilde{V}_k$, according as $(K-k)$ is even or odd, respectively $(k = 1, 2, \ldots, K)$.

At first sight it would appear that the above bounding properties must always be best possible, on the basis of the given information, since the bounding properties of $g_{K-P}(x)$ and $g^C_{K-P}(x)$ with respect to $G_K(x)$ are best possible. Such an argument was used in Sec. 4 to show that the bounding properties of $f_{N(P)+J}(x)$ and $f^C_{N(P)+J}(x)$ were best possible. However, to be rigorous, we must establish that these approximants are extremal series of Stieltjes. For example, this is readily seen to be true for $f_{N(P)+J}(x)$ and $f^C_{N(P)+J}(x)$: in much the same way as in Lemma 1 we find that $\mathcal{E}_{N(P)+J}(x)$ and $\mathcal{E}^C_{N(P)+J}(x)$ are both extremal series of Stieltjes, and then using (7) we find the same to be true for $f_{N(P)+J}(x)$ and $f^C_{N(P)+J}(x)$. In the present case it is found that the strengths of the poles of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$ corresponding to the fixed locations *are not necessarily all positive*. For example, we can consider without loss of generality the extremal series of Stieltjes

$$G^{\mathcal{E}}(x) = \frac{12}{(1+x)} + \frac{12}{(2+x)} + \frac{144}{(3+x)};$$

then corresponding to the set of information $\mathcal{E}_1 = 1$, $\mathcal{E}_2 = 2$, $G^{\mathcal{E}}(0) = 66$, $G^{\mathcal{E}}(1) = 46$, we obtain the approximant

$$g_{2+2(2)}(x) = \frac{-12}{(1+x)} + \frac{156}{(2+x)}.$$

Hence we cannot *generally* assert that the bounding properties of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$ are best possible on the basis of the given information. However, providing it turns out that all of the pole strengths of the approximants *are* positive, which often appears to be the case providing relatively few poles are fixed compared to the total number of pieces of given information, then indeed the bounding properties are best possible.

The reason that these negative pole strengths can occur is not hard to find. We simply note that the *entire derivation above, and the consequent bounding properties, remain unaltered when we lift the restriction* $V_k > 0$ $(k = 1, 2, \ldots, K)$, *and allow some or all of these strengths to be negative or vanish.* No reference was ever made to the positivity of these strengths: all we needed to know was that $G_K(x)$ was a series of Stieltjes. Thus there is no *a priori* reason to suppose that the corresponding strengths of the approximants should be positive.

We now note that the poles of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$ whose locations are not fixed, are located in $(-\infty, -R']$ and have positive strengths, since the same is true for $g_{K-P}(x)$ and $g^C_{K-P}(x)$, and by using (28). Hence, in general, we can say that the bounding properties of $g_{K+P(P)}(x)$ and $g^C_{K+P(P)}(x)$ with respect to $G(x)$ *are best possible, on the basis of the given information, providing that we replace the assertion* "$V_k > 0$" *by* "$-\infty < V_k < +\infty$" $(k = 1, 2, \ldots, K)$ *in* (9). For, if this is the case, the approximants are then indeed extremal forms of $G(x)$ and match all of the given information about $G(x)$.

The above results remain true when the more general set of N pieces of information about $G(x)$ at P points, $N \geq P$, is used. This can be proven rigorously by following similar lines of reasoning to those given above. The bounding properties of the resulting approximants $g_{K+N(P)}(x)$ and $g^C_{K+N(P)}(x)$, as defined in (22) and (23), are most easily seen by using the limiting case argument given in Sec. 2. We find that the bounding properties of $g_{K+N(P)}(x)$ and $g^C_{K+N(P)}(x)$ are the same as those of $g_{K+N(N)}(x)$ and $g^C_{K+N(N)}(x)$ in the limit where we let the first N_1 points $x_1, x_2, \ldots, x_{N_1}$ tend to coincidence at x_1, the next N_2 points tend to coincidence at x_2, and so on. In particular, the bounding properties in the region of the poles are unaltered. As an example, in Figure 5 we have sketched the bounding relationship between a typical $g_{3+4(3)}(x)$, its complement $g^C_{3+4(3)}(x)$, and $G(x) = \sum_{k=1}^{3} V_k/(\mathcal{E}_k + x) + H(x)$.

If the N pieces of given information are associated with the single point $x = 0$ and we know the locations of the first N poles, then the approximant $g_{N+N(1)}(x)$ is precisely the continued factorization approximant which was obtained by Tang[20] to bound the dynamical polarizability. To derive bounds complementary to those supplied by this approximant, Tang incorporates two[21] additional pieces of information relating to the behavior of the dynamical polarizability as $x \to \infty$. If we use the obvious generalization of our notation (recall Sec. 4), then we can denote this approximant by $g_{(N-1)+N(1)+2}(x)$. The bounds supplied by this approximant are then seen to be the same as those given by the $g_{(N-1)+N(1)}(x)$ which omits to use the information at infinity. This is what one would expect in view of the relationship between the bounding properties of an $f_{N(P)+J}(x)$ and the corresponding $f_{N(P)}(x)$ (recall Sec. 4).

We note that the present results are applicable for the dynamical polarizability function of an atom or molecule in an excited state. If the system is in its Kth excited state, then the dynamical polarizability can be written in the form of $G(x)$ in (9), except that $V_1, V_2, \ldots, V_K$ are now all negative. Providing the transition energies for these first K poles are known, together with an appropriate set of $N \geq K$ pieces of information at P points, then one can obtain bounds on the excited state polarizability at both real and imaginary frequencies.

7. CONCLUSION

In this paper we have seen how the multipoint Padé approximants, like the usual $[n, n-1]$ and $[n, n]$ Padé approximants, achieve the approximate analytic continuation of those functions which can be represented by a series of Stieltjes. The information which an approximant uses is very incomplete: It relates to the behavior of the function in a limited region and consists only of the first few terms in the Taylor series expansion of the function about each of a set of points. Even if these expansions had been known completely, their radii of convergence would all be bounded. The approximant describes the corresponding series of Stieltjes for all $x \in (-R, \infty)$, where R is the radius of convergence of the series of Stieltjes, by imposing rigorous bounds on it, both inside and outside the region defined by the radii of convergence associated with the given information. The approximant is itself an extremal series of Stieltjes, its form being essentially the same as the function which it seeks to approximate. Instead of having infinitely many (possibly a continuum of) positive simple poles located in $(-\infty, -R)$, the approximant has only a finite set. Furthermore, the multipoint Padé approximant "matches" all of the given information about the series of Stieltjes, and hence it falls into the category of "A Best Possible Approximation (On the Basis of the Given Information)." That is, on the basis of the given information alone, one cannot *know* that the true series of Stieltjes does not, in fact, lie arbitrarily close to the approximant, on any interval of interest. In particular, the bounds imposed by the approximant are best possible.

We have further seen how the multipoint Padé approximant can be made to incorporate additional information about the series of Stieltjes. Inclusion of (a lower bound to) the radius of convergence of the series of Stieltjes produces the complementary multipoint Padé approximant. This too is an extremal series of Stieltjes. The bounds which it supplies are an exact complement to those given by the original approximant, and they are best possible. Since the complementary approximant incorporates one additional piece of information one would expect that, over and above its bounding properties, it is a better *approximation* to the series of Stieltjes. We have also seen how information pertaining to the behavior of the series of Stieltjes as $x \to \infty$ can be built into the multipoint Padé approximant and its complement, thereby further tightening the bounds which they supply. Their nature as extremal series of Stieltjes remains unaltered and their bounding properties are still best possible (on the basis, now, of a larger set of given information).

However, the most important point about these approximants is that they constitute best possible approximations for the function which they seek to approximate. This is highlighted by our examination in Secs. 5 and 6 In Sec. 5 we established the various bounding properties of the multipoint Padé approximant and its complement in the region of poles, when the series of Stieltjes pos-

sesses a set of discrete poles whose exact locations are unknown. In particular, we saw how the approximant may often place its poles in the intervals between the discrete poles of the series of Stieltjes. It does so with a pleasing regularity, never putting more than one pole in any of these intervals, and thus emulates the *distribution* of the discrete poles as best it can with the limited set of information available. Indeed, in Sec. 6 we found that, by fixing the locations of some of the poles of the approximants at the true locations of the first few discrete poles of the series of Stieltjes, one can usually obtain best possible upper and lower bounds on the strengths of the discrete poles. More generally, by relaxing the condition that the first few poles of the "series of Stieltjes" be positive, we found that the corresponding approximants would then always yield a complementary pair of best possible bounds both outside and *inside* the region of the discrete fixed poles. Thus, we see that the inclusion of additional information in most cases leads not only to improved bounds, but also to a better approximation for the "series of Stieltjes" being considered.

This leads us to consider the multipoint Padé approximants to functions which are not series of Stieltjes. The above observations make one suspect that in dealing with any function whose behavior is largely dictated by its poles, various in their signs, orders, and locations, then given sufficient information the corresponding multipoint Padé approximant would still be a good approximation to the true function. Certainly, if the behavior of the function is defined solely by a finite or infinite set of *positive simple* poles then a very satisfactory way to proceed is to use the Padé approximant method. If information at one point is available (obtained from a perturbation expansion, for example) then the usual one-point Padé approximants should be tried as a means for analytically continuing the function. If information at more than one point is available (obtained possibly from experimental measurements), then a multipoint Padé approximant should be used. Regardless of possible bounding properties, one could at least always ensure that the resulting approximant is a *best possible approximation* to the true function. That is, one could ensure not only that the approximant matches the given information but also that it is of the correct functional form. If one could assert that the approximant is not best possible then one would necessarily be in possession of additional information: This too should be incorporated into the approximant, thereby overruling any such objection.

The above remarks are kindred to the Padé conjecture[13] for the usual one-point Padé approximants, and the related considerations of the general problem of rational approximation.[9,11]

ACKNOWLEDGMENTS

The author thanks Professor S. T. Epstein for his advice and assistance and Professor P. R. Certain for his encouragement. Thanks are also due to the referee for suggesting that consideration be made of fixing the locations of the poles.

*This research was supported by the National Science Foundation Grant GP-28213.

[1]For recent applications of the (usual) two-point Padé approximant method to functions not explicitly established to be series of Stieltjes, see, for example, A. Isihara and E. Montroll, Proc. Natl. Acad. Sci. USA **68,** 3111 (1971); P. Sheng and J. D. Dow, Phys. Rev. B **4,** 1343 (1971).

[2]For an application of the (usual) two-point Padé approximant method to a function which *is* a series of Stieltjes, see, for example, K. T. Tang, Phys. Rev. A **4,** 1033 (1971).

[3]For comprehensive references to the theory and applications of the Padé approximant method prior to 1970, see *The Padé Approximant in Theoretical Physics,* edited by G. A. Baker and J. L. Gammel (Academic, New York, 1970).

[4](Reference GB) G. A. Baker, J. Math. Phys. **10,** 814 (1969).

[5]This can be seen by immediate extensions of some recent work by G. Starkschall and R. G. Gordon, J. Chem. Phys. **54,** 663 (1971) in which a moment theoretical approach together with the linear programming method are used to obtain bounds on the dynamical polarizability, a well-known series of Stieltjes. The moment theory method as used here, and the methods of Secs. 2, 3, and 4 both yield best possible bounds on the basis of the given information, and hence both methods must be equivalent.

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[9]J. L. Walsh, J. Approx. Theory **3,** 236 (1970).

[10]A multipoint Padé approximant is a rational approximation. For discussion of the general problem of rational approximation see, for example, Refs. 9 and 11.

[11]J. Meinguet, *Approximation Theory,* edited by A. Talbot (Academic, New York, 1970), pp. 137–65.

[12]There are at least two methods by which such approximants could actually be calculated: (i) by setting up the approximant as a continued fraction and then obtaining the unknowns successively (cf. GB); (ii) by direct solution of the set of linear equations $A_N^{(n)}(X_m) - \Sigma_{l=0}^{n} \binom{n}{l} F^{(n)}(X_m) B_N^{(n-m)}(X_m) = 0, n = 0, 1, \ldots, N_m - 1, m = 1, 2, \ldots, P$. If, however, the given information is not exact, having been obtained from experimental data for example, then a linear programming technique should probably be used in order to ensure that the given information does indeed correspond to a series of Stieltjes.

[13]G. A. Baker, Jr., Advan. Theor. Phys. 1, 1 (1965).

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[15]To see this we note that $A_p(x)/B_p(x) > 0$ for $x \in (-R, \infty)$, as shown in Sec. 1. Moreover, $B_p(0)=1$. Thus we need only to show that $A_p(x)$ and $B_p(x)$ have no common factors. This is assured because the continued fraction expansion of $A_p(x)/B_p(x)$ [obtained by setting $F_p(x) \equiv 0$ in (3)] is unique and $a_1 > 0, a_2 > 0, \ldots, a_p > 0$.

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[21]Tang uses the coefficient of $(1/\omega^2)$ in the expansion of $\alpha(\omega^2)$ in inverse powers of ω^2. However, it is implicit in his procedure that $\alpha(-\omega^2) \to 0$ as $\omega \to \infty$, and hence in our notation (Sec. 4) $J = 2$.

A variational approach to the theory of multipoint Padé approximants

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(Received 11 August 1972)

The existence and bounding properties of the various multipoint Padé approximants, and their complements, with respect to functions representable by series of Stieltjes, are established by using a generalized Hylleraas variational principle. The main discussion uses the phraseology of a typical frequency dependent polarizability function, and in an appendix the results are simply generalized.

1. INTRODUCTION

In this paper we use a variational principle to establish the existence and bounding properties of the multipoint Padé approximants for functions which can be represented by a series of Stieltjes. Previously, variational methods have been used to establish bounding properties,[1–3] and also certain convergence properties,[4,5] of the one-point Padé approximants.

Although our final objectives are fairly general, throughout the body of this paper we will examine these approximants in the context of a typical polarizability of a physical system[6] (more precisely, a typical diagonal multipole ground state polarizability). In Appendix C we will show how the variational arguments used to discuss this function can be generalized so that the theory becomes applicable to arbitrary functions which can be represented by a series of Stieltjes.[7]

By working with the example of a dynamical polarizability we serve two ends. First, a derivation in this context allows us to unify the various moment theoretical and one-point Padé approximant methods which have been used to bound such polarizabilities.[8] Second, it provides a simple example from which the corresponding generalized results pertaining to arbitrary series of Stieltjes can be more easily understood.

The theory of the multipoint Padé approximants can also be derived using more classical methods; continued fractions,[9] or moment theory.[10,11] However, the variational formulation provides a complementary point of view: Namely, in the classical approaches one starts with an assumed analytic form for the approximant and the goal is then to establish its bounding properties. On the other hand, in the variational approach one starts with a general bound and the goal is to show that, by proper selection of a trial function, one can obtain the desired form for the approximant. It is thus not surprising that some aspects may be seen more directly from one point of view than from the other. More subjectively, to one with some knowledge of the Rayleigh–Ritz method, the mathematical manipulations in the variational approach will be seen to be quite straightforward and, in particular, to involve no heavy algebra.

We will denote a typical polarizability by $B(\omega^2)$ where ω is a real or imaginary frequency. For simplicity of discussion we will replace ω^2 by the real variable $-x$. Thus $B(x)$ for $x<0$ is the polarizability at real frequencies, and for $x>0$ it is the polarizability at imaginary frequencies. Then if $E_{10}=E_1-E_0$ denotes the first excitation energy for the system under consideration, $B(x)$ is a well-defined analytic function of x for $-E_{10}^2<x<\infty$, and possesses poles lying on the negative real axis at points $-\infty<x\leq -E_{10}^2$. Their locations correspond to the excitation energies of the system, and we will refer to their (positive) residues in a general way as oscillator strengths. (This assumes that our system possesses only bound states. In actual fact there are inevitably continua, with their associated cuts, but since this only complicates the notation and not the analysis we will not introduce this extra complication.)

Let us now suppose that we are given the information

$$B^{(n)}(x_p) \text{ for } \begin{cases} n=0,1,\ldots,N_p-1, & N_p\geq 1 \\ p=1,2,\ldots,Q \end{cases} \tag{1}$$

with

$$\sum_{p=1}^{Q} N_p = N$$

and

$$-E_{10}^2<x_1<x_2<\cdots<x_Q<\infty;$$

and where

$$B^{(n)}(x_p)\equiv \frac{d^nB(x)}{dx^n}\Big|_{x=x_p}.$$

Thus, we are given N pieces of information about $B(x)$, associated with Q points. In Sec. 2 we will first show how such a set of information can be used to construct a variationally optimal approximant to $B(x)$ which matches $B(x)$ at the data points and which provides rigorous bounds on $B(x)$ elsewhere in the region $-E_{10}^2<x<\infty$. We will then show that this approximant is in fact $B_{N(Q)}(x)$, the multipoint Padé approximant to $B(x)$ which corresponds to the given set of information. For simplicity we will begin by considering the case where $N=Q$, so that there is only one piece of information at each point x_p $(p=1,2,\ldots,Q)$, and then use a limiting argument to extend the results to the general case. In Sec. 3 we show how, by using one additional piece of information, namely the first excitation energy E_{10}, we can obtain the complementary multipoint Padé approximant $B^c_{N(Q)}(x)$. The bounds which it supplies are the exact complement to those supplied by the original approximant $B_{N(Q)}(x)$. In the case that all of the given information relates to the single point $x=0$ the corresponding multipoint Padé approximant $B_{N(1)}(x)$ becomes either an $[n,n-1]$ or $[n,n]$ one-point Padé approximant to $B(x)$, and the bounding properties of these usual[7,12] approximants are seen as a special case. In Appendix A the limiting arguments used in Secs. 2 and 3 are given a rigorous mathematical foundation by extending the variational derivation used in the case $N=Q$.

In Sec. 4 we show how "high frequency information" in the form of the first few terms in the series expansion of $B(x)$ in powers of $(1/x)$ can be built into the approximants, thereby tightening the complementary pair of bounds supplied by $B_{N(Q)}(x)$ and $B^c_{N(Q)}(x)$. The two-point Padé approximants as used by Tang[13] to bound the dipole polarizability are demonstrated to occur as a special case of following this procedure.

In Sec. 5 we consider briefly a family of nonoptimal multipoint Padé approximants to $B(x)$. These reduce, in the case of information only at the one point $x = 0$, to the $[n-k, n+k]$ and $[n-k, n+k-1]$ ($k = 1, 2, \ldots, n-1$ or n), one-point Padé approximants,[7] and thus they are of interest in connection with the Padé Table for multipoint approximants,[14] and with the general problem of rational approximation.[15]

2. THE MULTIPOINT PADÉ APPROXIMANT $B_{N(Q)}(x)$ TO $B(x)$

Let ψ_n and E_n denote, respectively, the normalized eigenfunctions and eigenvalues of a Hamiltonian H_0, with ψ_0 the ground state, and let V be some self-adjoint operator. Then $B(x)$ has the general form

$$B(x) = \sum_n{}' \frac{b_{0n}}{(E_{n0}^2 + x)}, \tag{2}$$

where $E_{n0} = E_n - E_0$ and where b_{0n} is an "oscillator strength"

$$b_{0n} = E_{n0}(\psi_0, V\psi_n)(\psi_n, V\psi_0) > 0.$$

In accord with the discussion of Sec. 1 we now suppose that we are given the information

$$B(x_p) \quad \text{for} \quad p = 1, 2, \ldots, Q \tag{3}$$

where

$$-E_{10}^2 < x_1 < x_2 < \cdots < x_Q < \infty.$$

Let us define the function

$$\sqrt{b} = \sum_n b_{0n}^{1/2}\psi_n \tag{4}$$

so that we can write

$$B(x_p) = (\sqrt{b}, [(H_0 - E_0)^2 + x_p]^{-1}\sqrt{b}), \quad p = 1, 2, \ldots, Q. \tag{5}$$

Then we observe the algebraic identity

$$B(x) = \beta(Q-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)\gamma(x) \tag{6}$$

where

$$\beta(Q-1; x) = \sum_{p=1}^{Q}\left(\prod_{p=1}^{Q}{}' \frac{(x_p - x)}{(x_p - x_q)}\right) B(x_p)$$

is the unique polynomical of degree $(Q-1)$ which satisfies

$$\beta(Q-1; x_p) = B(x_p), \quad p = 1, 2, \ldots, Q;$$

and where

$$\gamma(x) = \sum_n{}' \frac{b_{0n}}{(E_{n0}^2 + x_1)(E_{n0}^2 + x_2)\cdots(E_{n0}^2 + x_Q)(E_{n0}^2 + x)}$$
$$= (\sqrt{b}, [(H_0 - E_0)^2 + x_1]^{-1}\cdots[(H_0 - E_0)^2 + x_Q]^{-1} \times [(H_0 - E_0)^2 + x]^{-1}\sqrt{b}).$$

This separation has the result of allowing us to concentrate on $\gamma(x)$ secure in the knowledge that any [but see following Eq. (15) below] approximation to $B(x)$ produced by an approximation to $\gamma(x)$ will be consistent with the given information since the coefficient of $\gamma(x)$ vanishes at each information point.

If now we introduce the generalized Hylleraas functional[16]

$$\tilde{\gamma}(x) = -(\tilde{\Phi}, [(H_0 - E_0)^2 + x_1]\cdots[(H_0 - E_0)^2 + x_Q] \times [(H_0 - E_0)^2 + x]\tilde{\Phi}) + (\tilde{\Phi}, \sqrt{b}) + (\sqrt{b}, \tilde{\Phi}), \tag{7}$$

then it is easy to prove that

$$\tilde{\gamma}(x) \leq \gamma(x) \quad \text{for} \quad -E_{10}^2 < x < \infty$$

providing the trial function $\tilde{\Phi}$ satisfies

$$(\tilde{\Phi}, \psi_0) = 0. \tag{8}$$

Suppose now that we have *any* such lower bound $\tilde{\gamma}(x)$ to $\gamma(x)$. On substitution into Eq. (6) we obtain an approximation to $B(x)$,

$$\tilde{B}(x) = \beta(Q-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)\tilde{\gamma}(x), \tag{9}$$

whose bounding properties are easily seen by comparison with Eq. (6) to be

$$\begin{aligned} &\tilde{B}(x) \leq B(x) \quad \text{for} \quad -E_{10}^2 < x < x_1, \\ &\tilde{B}(x) \geq B(x) \quad \text{for} \quad x_1 < x < x_2, \\ &\tilde{B}(x) \leq B(x) \quad \text{for} \quad x_2 < x < x_3, \\ &\cdots \qquad\qquad \cdots \end{aligned} \tag{10}$$

$\tilde{B}(x) \geq$, or $\leq$, $B(x)$ for $x_Q < x < \infty$, according as Q is odd, or even, respectively.

Thus, by using a variational trial function in Eq. (7), chosen so that the only inner products which occur are of the form (5), we can obtain an approximant to $B(x)$ which agrees with $B(x)$ at the data points, utilizes only the given information (3), and displays the bounding properties (10).

One then finds, by induction from $Q = 1, 2, 3\ldots$, that seemingly the most flexible trial function of the desired form is

$$\tilde{\Phi} = \sum_{r=1}^{[Q/2]} a_r (H_0 - E_0)^{2r-2}\left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-1}\right)\sqrt{b}, \tag{11}$$

where $a_1, a_2, \ldots, a_{[Q/2]}$ are variational parameters and where $[R]$ denotes the integer part of R. It is readily verified that this trial function satisfies Eq. (8).

On substitution into Eq. (7) we obtain

$$\tilde{\gamma}(x) = -\sum_{r=1}^{[Q/2]}\sum_{s=1}^{[Q/2]} c_{rs}(x) a_r^* a_s + \sum_{r=1}^{[Q/2]} d_r(a_r + a_r^*), \tag{12}$$

where

$$c_{rs}(x) = \left(\sqrt{b}, (H_0 - E_0)^{2(r+s)-4}[(H_0 - E_0)^2 + x] \times \left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-1}\right)\sqrt{b}\right)$$
$$= \sum_{p=1}^{Q}(-x_p)^{r+s-2}(x - x_p)\left(\prod_{q=1}^{Q}{}' (x_q - x_p)^{-1}\right) B(x_p)$$

and

$$d_r = \left(\sqrt{b}, (H_0 - E_0)^{2r-2}\left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-1}\right)\sqrt{b}\right)$$
$$= \sum_{p=1}^{Q}(-x_p)^{r-1}\left\{\prod_{q=1}^{Q}{}'(x_q - x_p)^{-1}\right\}B(x_p).$$

Here it is seen that, as desired, only the known scalars x_p and inner products $B(x_p)(p = 1, 2, \ldots, Q)$ occur.

The optimal choice $\hat{a}$ of the a's is obtained by requiring that

$$\frac{\partial\tilde{\gamma}(x)}{\partial a_r^*} = 0 \quad \text{for} \quad r = 1, 2, \ldots, [Q/2]$$

which yields the set of conditions

$$\sum_{s=1}^{[Q/2]} c_{rs}(x)\hat{a}_s = d_r, \quad r = 1, 2, \ldots, [Q/2].$$

By using Cramer's rule we find that

$$\hat{a}_s = \frac{\begin{vmatrix} c_{11}(x) & \cdots & c_{1(s-1)}(x) & d_1 & c_{1(s+1)}(x) & \cdots & c_{1[Q/2]}(x) \\ c_{21}(x) & \cdots & c_{2(s-1)}(x) & d_2 & c_{2(s+1)}(x) & \cdots & c_{2[Q/2]}(x) \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot & \cdot & & \cdot \\ c_{[Q/2]1}(x) & \cdots & c_{[Q/2](s-1)}(x) & d_{[Q/2]} & c_{[Q/2](s+1)}(x) & \cdots & c_{[Q/2][Q/2]}(x) \end{vmatrix}}{\begin{vmatrix} c_{11}(x) & c_{12}(x) & \cdots & c_{1[Q/2]}(x) \\ c_{21}(x) & c_{22}(x) & \cdots & c_{2[Q/2]}(x) \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ c_{[Q/2]1}(x) & c_{[Q/2]2}(x) & \cdots & c_{[Q/2][Q/2]}(x) \end{vmatrix}},$$

and it is easy to show that the corresponding optimized $\tilde{\gamma}(x)$ is

$$\hat{\gamma}(x) = \sum_{s=1}^{[Q/2]} d_s\hat{a}_s.$$

In particular, we note that each of the $c_{rs}(x)$ is linear in x and that the d_r are independent of x. Hence we write

$$\hat{\gamma}(x) = \frac{\text{polynomial in } x \text{ of degree } [Q/2]-1}{\text{polynomial in } x \text{ of degree } [Q/2]} = \frac{R([Q/2]-1; x)}{S([Q/2]; x)}, \quad (13)$$

where the coefficients are expressed in terms of the given information alone.

The corresponding approximant to $B(x)$ is denoted $\hat{B}(x)$, and it is obtained as in Eq. (9);

$$\hat{B}(x) = \beta(Q-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)\hat{\gamma}(x) \quad (14)$$
$$= \frac{\beta(Q-1; x)S([Q/2], x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)R([Q/2]-1; x)}{S([Q/2]; x)}$$

The bounding properties of $\hat{B}(x)$ with respect to $B(x)$ must be exactly the same as those tabulated in Eq. (10) for $\tilde{B}(x)$.

We will now establish two points about $B(x)$; we will show that

$$\hat{B}(x_p) = B(x_p) \quad \text{for} \quad p = 1, 2, \ldots, Q \quad (15)$$

and that the degree of the polynomial in the numerator of Eq. (14) is in fact $[(Q-1)/2]$, so that $B(x)$ can be written

$$B(x) = \frac{\text{polynomial in } x \text{ of degree } [(Q-1)/2]}{\text{polynomial in } x \text{ of degree } [Q/2]}. \quad (16)$$

We compare Eqs. (15) and (16) with the case $N = Q$ in the following definition: Given the set of information Eq. (1), the corresponding multipoint Padé approximant $B_{N(Q)}(x)$ is defined[9] as

$$B_{N(Q)}(x) = a_N(x)/b_N(x), \quad (17)$$

where $a_N(x)$ and $b_N(x)$ are the polynomials of degrees $[(N-1)/2]$ and $[N/2]$, respectively, which are uniquely specified by the set of conditions

$$B^{(n)}_{N(Q)}(x_p) = B^{(n)}(x_p) \text{ for } \begin{cases} n = 0, 1, \ldots, Np-1 \\ p = 1, 2, \ldots, Q \end{cases} \quad (18)$$

together with a normalization requirement, say

$$b_N(0) = 1.$$

We conclude from the evident uniqueness of this approximant (assuming that it exists!) that we must, in fact, have $\hat{B}(x) = B_{Q(Q)}(x)$. Thus, by proving Eqs. (15) and (16) we will establish the *existence of the approximant* $B_{Q(Q)}(x)$, and we will establish that *it displays the bounding properties attributed to* $\tilde{B}(x)$ *in Eq. (10).*

We note that Eq. (15) follows immediately providing that the polynomial occurring in the denominator of $\hat{\gamma}(x)$, $S([Q/2]; x)$, has no factors in common with $\prod_{p=1}^{Q}(x_p - x)$. To see that this is the case we observe that

$$S([Q/2]; x) = \det|(\phi_i, [(H_0 - E_0)^2 + x]\phi_j)|, \quad i, j = 1, 2, \ldots, [Q/2],$$

where

$$\phi_i = \left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-1/2}\right)(H_0 - E_0)^{2i-2\sqrt{b}} \quad (19)$$

Therefore the equation $S([Q/2]; -x) = 0$ is precisely the characteristic equation which one would obtain if the set of functions (19) was used as a linear variational basis in a Rayleigh–Ritz procedure for finding approximations $-x$ to the eigenvalues $E_{i0}^2 (i = 1, 2, \ldots, [Q/2])$

of $(H_0 - E_0)^2$. Since these roots of $S([Q/2]; -x)$ are well known to upper bound the E^2_{10}, it follows that the roots of $S([Q/2]; x)$ are successive lower bounds to the numbers $-E^2_{10}, -E_{20}, \ldots, -E^2_{[Q/2]\,0}$. Further, if instead of using the ϕ_i as a basis set we equivalently use those orthornormal linear combinations of the ϕ_i which diagonalize $(H_0 - E_0)^2$, then it is clear that $\hat{\gamma}(x)$ can be written in the form

$$\hat{\gamma}(x) = \sum_{n=1}^{[Q/2]} \frac{d_{0n}}{(\hat{E}^2_{n0} + x)}, \tag{20}$$

where the d_{0n} are finite *positive* numbers and the $\hat{E}^2_{n0}$ are the variational upper bounds to the E^2_{n0} described above.[17] However, at this point if suffices to notice that the roots of $S([Q/2]; x)$ are located in $-\infty < x \leq -E^2_{10}$, and hence not in the region of the x_p. Thus we are assured that Eq. (15) is indeed true.

To prove Eq. (16) we note first that the new functional

$$\xi(x) = -(\tilde{\theta}, [1 + (1/x)(H_0 - E_0)^2]\tilde{\theta}) + (\tilde{\theta}, W^{-1/2}\sqrt{b}) + (W^{-1/2}\sqrt{b}, \tilde{\theta}), \tag{21}$$

where

$$W = [(H_0 - E_0)^2 + x_1][(H_0 - E_0)^2 + x_2] \times \cdots [(H_0 - E_0)^2 + x_Q],$$

is related to our original functional (7) through the statement

$$\tilde{\theta} = xW^{1/2}\tilde{\Phi} \Rightarrow \xi(x) = x\tilde{\gamma}(x).$$

Furthermore, it is clear that $\tilde{\gamma}(x)$ is stationary with respect to variations of the linear trial function $\tilde{\Phi}$ about $\hat{\Phi}$ iff $\xi(x)$ is stationary with respect to the variations of $\tilde{\theta} = xW^{1/2}\tilde{\Phi}$ about $\hat{\theta} = xW^{1/2}\hat{\Phi}$. Hence we can discuss our variational procedure in terms of the functional (21).

We now note that $\xi(x)$ attains the exact value $x\gamma(x)$ when we use the formally expanded trial function

$$\theta_{\text{exact}} = \sum_{n=0}^{\infty} \left(\frac{1}{x}\right)^n (H_0 - E_0)^{2n} W^{-1/2}\sqrt{b}$$

and hence the trial function $\tilde{\theta} = xW^{1/2}\tilde{\Phi}$ corresponding to our choice (11) is such that it *could* agree with θ_{exact} through the term in $(1/x)^{[Q/2]-1}$. The variational principle then ensures that $\hat{\theta} = xW^{1/2}\hat{\Phi}$ *is* indeed this accurate,[18] and since the error in $x\hat{\gamma}(x)$ is second order in the error in $\hat{\theta}$ it follows that $x\hat{\gamma}(x)$ is accurate through the term in $(1/x)^{2[Q/2]-1}$. Hence $\hat{\gamma}(x)$ must agree with $\gamma(x)$ through the term in $(1/x)^{2[Q/2]}$.

It now follows that

$$B(x) - \hat{B}(x) = \left(\prod_{p=1}^{Q} (x_p - x)\right)[\gamma(x) - \hat{\gamma}(x)]$$

$$= O((1/x)^{2[Q/2]+1-Q})$$

$$= \begin{cases} O((1/x)^0) & \text{if } Q \text{ is odd} \\ O((1/x)^1) & \text{if } Q \text{ is even} \end{cases}.$$

Hence, since $\lim B(x) = 0$, as $x \to \infty$, we have

$$\lim_{x\to\infty} \hat{B}(x) = \begin{cases} \text{const} & \text{if } Q \text{ is odd} \\ 0 & \text{if } Q \text{ is even} \end{cases},$$

and thus the polynomial in the numerator of Eq. (14) must in fact be of degree *at most* $[\frac{1}{2}(Q-1)]$. To see that this is *exactly* the degree of the polynomial we consider the cases Q even and Q odd separately.

Q even: Using Eq. (20) in Eq. (14), we write $\hat{B}(x)$ as

$$\hat{B}(x) = \beta(Q-1; x) + \left(\prod_{p=1}^{Q} (x_p - x)\right) \sum_{n=1}^{[Q/2]} \frac{d_{0n}}{(\hat{E}^2_{n0} + x)}$$

The coefficient of $(1/x)$ in the expansion of this expression can only arise from the last term here and is found to be

$$\sum_{n=1}^{[Q/2]} d_{0n} \left(\prod_{p=1}^{Q} (x_p + \hat{E}^2_{n0})\right) > 0,$$

whence in the case that Q is even we deduce that the degree of the polynomial in the numerator of Eq. (14) is exactly $[(Q-1)/2]$:

Q odd: Here we show that $\hat{B}(x) \not\to 0$ as $x \to \infty$. From Eq. (21) we have

$$x\gamma(x) - x\hat{\gamma}(x) = ((\theta_{\text{exact}} - \hat{\theta}), [1 + (1/x)(H_0 - E_0)^2](\theta_{\text{exact}} - \hat{\theta}))$$

and providing we are dealing with a system for which infinitely many of the oscillator strengths are nonzero [this is certainly true when $B(x)$ is representable by a series of Stieltjes: see Appendix C] so that $\theta \neq \theta_{\text{exact}}$, it is clear that the leading term in this error, which is of order $(1/x)^{2[Q/2]}$, cannot vanish, whence $\lim \hat{B}(x) \neq 0$ as $x \to \infty$ as desired.

This completes the proof of the existence and bounding properties of $B_{Q(Q)}(x)$. We now turn our attention to the general case of a $B_{N(Q)}(x)$ multipoint Padé approximant to $B(x)$, defined in Eqs. (17) and (18). Does such an approximant exist for $N > Q$? What are its bounding properties?

The answers to both of these questions are immediate when one sees that a $B_{N(Q)}(x)$ can always be realized as a limiting case of a $B_{N(N)}(x)$. We start with the $B_{N(N)}(x)$ corresponding to the set of N pieces of information $B(x'_p)$ $(p = 1, 2, \ldots, N)$ where $-E^2_{10} < x'_1 < x'_2 < \cdots < x'_N < \infty$. We already know that this approximant exists, and that it is of the form (17). Now let the first N_1 points $x'_1, x'_2, \ldots, x'_{N_1}$ tend to coincidence at x_1, let the next N_2 points $x'_{N_1+1}, x'_{N_1+2}, \ldots, x'_{N_1+N_2}$ tend to coincidence at $x_2, \ldots$, the remaining N_Q points $x'_{N-N_Q+1}, x'_{N-N_Q+2}, \ldots, x'_N$, tend to coincide at x_Q. The resulting approximant, which for simplicity we will still denote by $\hat{B}(x)$, remains in the form (17). Furthermore, it is clear that $B(x) - \hat{B}(x)$ will now have a zero of multiplicity N_1 at x_1, N_2 at $x_2, \ldots, N_Q$ at x_Q, and hence

$$B^{(n)}(x_p) = B^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases}.$$

Comparing this with Eq. (18) we deduce that $\hat{B}(x) \equiv B_{N(Q)}(x)$. In particular, the bounding properties of $B_{N(Q)}(x)$ with respect to $B(x)$ are a direct consequence of the bounding properties of $B_{N(N)}(x)$ and the limiting process

described above. The bounding properties of $B_{N(Q)}(x)$ are thus

$$B_{N(Q)}(x) \leq B(x) \quad \text{for} \quad -E_{10}^2 < x < x_1,$$

$$B_{N(Q)}(x) \geq, \text{or} \leq, B(x) \quad \text{for} \quad x_1 < x < x_2,$$

according as N_1 is odd, or even, respectively; (22)

$$B_{N(Q)}(x) \geq, \text{or} \leq, B(x) \quad \text{for} \quad x_2 < x < x_3,$$

according as $N_1 + N_2$ is odd, or even, respectively;

$$B_{N(Q)}(x) \geq, \text{or} \leq, B(x) \quad \text{for} \quad x_Q < x < \infty,$$

according as $N_1 + N_2 \cdots + N_Q = N$ is odd, or even, respectively.

To actually obtain the approximants $B_{Q(Q)}(x)$ and, in general, $B_{N(Q)}(x)$, one of course does not follow the elaborate procedures described above. In practice one starts with Eqs. (17) and (18) and then solves the corresponding linearized problem.[19]

In Appendix A we rederive the above results rigorously by generalizing the variational arguments used at the beginning of this section.

For the special case that all of the given information (1) is associated with the single point $x = 0$, the multipoint Padé approximant becomes the usual $[n, n-1]$ or $[n, n]$ one-point Padé approximant,[7] and can be denoted by $B_{N(1)}(x) = [[N/2], [(N-1)/2)]]$ in the customary notation. The well-known bounding properties[7,12] of these approximants are now seen as a limit of those of the general multipoint Padé approximant.

3. THE COMPLEMENTARY MULTIPOINT PADÉ APPROXIMANT $B^c_{N(Q)}(x)$ TO $B(x)$

We assume now that in addition to the given information (1) we also know the number E_{10}.[20] The complementary multipoint Padé approximant to $B(x)$ is associated with this now larger set of given information, and it is defined as the function[9]

$$B^c_{N(Q)}(x) = c_N(x)/d_N(x), \tag{23}$$

where $c_N(x)$ and $d_N(x)$ are the polynomials of degrees $[N/2]$ and $[(N+1)/2]$, respectively, which are uniquely specified by the set of conditions

$$(B^c_{N(Q)})^{(n)}(x_p) = B^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases} \tag{24}$$

together with the two requirements

$$d_N(0) = 1 \quad \text{and} \quad d_N(-E_{10}^2) = 0. \tag{25}$$

The latter equation serves to place a pole of the approximant at $x = -E_{10}^2$.

We will establish the existence of this approximant and prove that the bounds which it supplies are the exact complement to those given by the original approximant $B_{N(Q)}(x)$, by using arguments analogous to those of Sec. 2. We begin by considering the case $N = Q$ as before.

We now rewrite $B(x)$ in Eq. (2) so as to separate out a pole term, thus

$$B(x) = (E_{10}^2 + x)^{-1}\Big((E_{10}^2 + x_1)B(x_1) + (x - x_1)\sum_n{}' \frac{(E_{n0}^2 - E_{10}^2)b_{0n}}{(E_{n0}^2 + x_1)(E_{n0} + x)}\Big)$$

$$= (E_{10}^2 + x)^{-1}[(E_{10}^2 + x_1)B(x_1) + (x - x_1)B'(x)], \tag{26}$$

where

$$B'(x) = \sum_n{}' \frac{b'_{0n}}{(E_{n0}^2 + x)}$$

$$\text{with } b'_{0n} = (E_{n0}^2 - E_{10}^2)b_{0n}/(E_{n0}^2 + x_i).$$

Here $B'(x)$ has the same form as $B(x)$ in Eq. (2), and we can rewrite it as

$$B'(x) = (\sqrt{b'}, [(H_0 - E_0)^2 + x]^{-1}\sqrt{b'}),$$

where we have made the obvious generalization of the notation (4).

From Eq. (26) we have

$$B'(x) = [B(x)(E_{10}^2 + x) - B(x_1)(E_{10}^2 + x_1)]/(x - x_1),$$

and we can use this equation to transform the set of given information (1) in the case $N = Q$, into a set of $Q - 1$ pieces of information about $B'(x)$. That is, we can obtain the values of

$$B'(x_p) = (\sqrt{b'}, [(H_0 - E_0)^2 + x_p]^{-1}\sqrt{b'}) \text{ for } p = 2, 3, \ldots, Q. \tag{27}$$

The situation is thus seen to be almost analogous to that in Sec. 2, and it is not hard to guess how we will proceed. We write

$$B'(x) = \beta'(Q-2; x) + \Big(\prod_{p=2}^{Q}(x_p - x)\Big)\gamma'(x), \tag{28}$$

where $\beta'(Q-2; x)$ is the unique polynomial of degree $Q-2$ which satisfies $\beta'(Q-2; x_p) = B'(x_p)$ $(p = 2, 3, \ldots, Q)$ and where

$$\gamma'(x) = \sum_n{}' \frac{b'_{0n}}{(E_{n0}^2 + x_2)(E_{n0}^2 + x_3)\cdots(E_{n0}^2 + x_Q)(E_{n0}^2 + x)}$$

$$= (\sqrt{b'}, [(H_0 - E_0)^2 + x_2]^{-1}\cdots[(H_0 - E_0)^2 + x_Q]^{-1} \times [(H_0 - E_0)^2 + x]^{-1}\sqrt{b'}).$$

This expression should be compared with Eq. (6).

If we now introduce the functional

$$\tilde{\gamma}'(x) = -(\tilde{\Phi}', [(H_0 - E_0)^2 + x_2]\cdots[(H_0 - E_0)^2 + x_Q] \times [(H_0 - E_0)^2 + x]\tilde{\Phi}') + (\tilde{\Phi}', \sqrt{b'}) + (\sqrt{b'}, \tilde{\Phi}'), \tag{29}$$

then it is easy to prove that

$$\tilde{\gamma}'(x) \leq \gamma'(x) \quad \text{for} \quad -E_{20}^2 < x < \infty$$

providing the trial function $\tilde{\Phi}'$ satisfies

$$(\tilde{\Phi}', \psi_0) = 0.$$

Suppose now that we have any such lower bound $\tilde{\gamma}'(x)$ to $\gamma'(x)$. On substitution into Eq. (28) and of the resulting approximation for $B'(x)$ into Eq. (26), we obtain an approximant to $B(x)$:

$$\tilde{B}^c(x) = (E_{10}^2 + x)^{-1}\left((E_{10}^2 + x_1)B(x_1) + (x - x_1)\right.$$
$$\left.\times\left[\beta'(Q-2;x) + \left(\prod_{p=2}^{Q}(x_p - x)\right)\tilde{\gamma}'(x)\right]\right)$$

whose bounding properties are immediately seen to be

$$\begin{aligned}
&\tilde{B}^c(x) \leqslant B(x) \quad \text{for} \quad -E_{20}^2 < x < -E_{10}^2,\\
&\tilde{B}^c(x) \geqslant B(x) \quad \text{for} \quad -E_{10}^2 < x < x_1,\\
&\tilde{B}^c(x) \leqslant B(x) \quad \text{for} \quad x_1 < x < x_2,\\
&\quad\cdots \qquad\qquad\qquad\quad \cdots\\
&\tilde{B}^c(x) \leqslant, \text{or} \geqslant, B(x) \text{ for } x_Q < x < \infty,
\end{aligned} \tag{30}$$

according as Q is odd or even, respectively. We note that these bounds are complementary to those described in Eq. (10), together with an additional bound for $-E_{20}^2 < x < -E_{10}^2$.

In order to obtain a lower bound $\tilde{\gamma}'(x)$ to $\gamma'(x)$ which involves only the transformed set of information (27) we use the trial function

$$\Phi' = \sum_{r=1}^{[(Q-1)/2]} a'_r(H_0 - E_0)^{2r-2}\left(\prod_{p=2}^{Q}[(H_0 - E_0)^2 + x_p]^{-1}\right)\sqrt{b'}$$

in Eq. (29), where $a'_1, a'_2, \ldots, a'_{[(Q-1)/2]}$ are variational parameters. The reasoning now follows identical lines to that in Sec. 2. We end up with an approximant $\hat{B}'(x)$ to $B'(x)$ which can be written in the form

$$\hat{B}'(x) = a'_{Q-1}(x)/b'_{Q-1}(x),$$

where $a'_{Q-1}(x)$ and $b'_{Q-1}(x)$ are polynomials of degrees $[(Q-2)/2]$ and $[(Q-1)/2]$, respectively, whose coefficients involve only the known quantities $x_p, B'(x_p)$ $(p = 2, 3, \ldots, Q)$ as desired. Furthermore, this approximant satisfies

$$\hat{B}'(x_p) = B'(x_p), \qquad p = 2, 3, \ldots, Q,$$

and on substitution for $B'(x)$ in Eq. (26) we obtain an approximant to $B(x)$

$$\hat{B}^c(x) = (E_{10}^2 + x)^{-1}[(E_{10}^2 + x_1)B(x_1) + (x - x_1)\hat{B}'(x)]$$
$$= \frac{(E_{10}^2 + x_1)B(x_1)b'_{Q-1}(x) + (x - x_1)a'_{Q-1}(x)}{(E_{10}^2 + x)b'_{Q-1}(x)}$$
$$= \frac{\text{polynomial in } x \text{ of degree } [Q/2]}{\text{polynomial in } x \text{ of degree } [(Q+1)/2]},$$

where the coefficients of the polynomials can be expressed in terms of the given information (1), in the case $N = Q$, and the number E_{10}. It is easily seen that this approximant satisfies conditions (23), (24), and (25), in the case $N = Q$, and hence by the uniqueness we have $\hat{B}^c(x) \equiv B^c_{Q(Q)}(x)$. In particular, we have established the existence of the complementary multipoint Padé approximant $B^c_{Q(Q)}(x)$, and we have proved that it displays the bounding properties (30).

To see the existence and bounding properties of the complementary multipoint Padé approximant $B^c_{N(Q)}(x)$ in the general case $N > Q$, we used the same limiting argument as was given near the end of Sec. 2. In this way the bounding properties of $B^c_{N(Q)}(x)$ are easily visualized. The bounds imposed are seen to be complementary to those described in Eq. (22) for the $B_{N(Q)}(x)$ which utilizes the same set of given information, together with an additional lower bound, $B^c_{N(Q)}(x) \leqslant B(x)$ for $-E_{20}^2 < x < -E_{10}^2$. Further the limiting argument lends credibility to the existence of $B^c_{N(Q)}(x)$ and can be rigorously validated with a variational proof similar to that given in Appendix A.

The present demonstrations have served to establish the existence and bounding properties of $B^c_{N(Q)}(x)$: To actually obtain such an approximant one proceeds directly from the set of defining Eqs. (23), (24), and (25), in much the same way as is done for $B_{N(Q)}(x)$.[19]

In the special case that all of the given information corresponds to the single point $x = 0$ we obtain the approximant $B^c_{N(1)}(x)$. The latter has been described by Baker,[21] and the bounds which it imposes are the precise complement to those given by the usual $[[(N/2], [(N-1)/2]]$ one-point Padé approximant which uses the same set of information.

4. UTILIZATION OF COEFFICIENTS FROM THE EXPANSION OF $B(x)$ IN INVERSE POWERS OF x

Here we suppose that in addition to the given information (1) we also know the coefficients of the first few terms in the expansion of $B(x)$ in powers of $(1/x)$. That is, we have

$$B(x) \sim S(0)(1/x) - S(2)(1/x)^2 + \cdots + (-1)^{J+1}S(2J-2)(1/x)^J + \text{higher terms with unknown or divergent coefficients} \tag{31}$$

where evidently

$$S(-2j) = \sum_n{}' b_{0n}E_{n0}^{2j} = (\sqrt{b}, (H_0 - E_0)^{2j}\sqrt{b}),$$
$$j = 0, 1, \ldots, J-1, \qquad J \geqslant 1.$$

The multipoint Padé approximant associated with the set of information (1) and (31) is denoted $B_{N(Q)+J}(x)$. It is defined[9] by

$$B_{N(Q)+J}(x) = a_{N+J}(x)/b_{N+J}(x), \tag{32}$$

where $a_{N+J}(x)$ and $b_{N+J}(x)$ are the polynomials of degrees $[(N+J)/2] - 1$ and $[(N+J)/2$, respectively, which are uniquely specified by the requirements

$$(B_{N(Q)+J})^{(n)}(x_p) = B^{(n)}(x_p) \quad \text{for} \quad \begin{cases} n = 0, 1, \ldots, N_{p-1}, \\ p = 1, 2, \ldots, Q \end{cases} \tag{33}$$

$$B_{N(Q)+J}(x) \sim S(0)(1/x) - S(2)(1/x)^2 + \cdots + \begin{cases} (-1)^{J+1}S(2J-2)(1/x)^J \text{ if } N+J \text{ is even} \\ (-1)^J S(2J-4)(1/x)^{J-1} \text{ if } N+J \text{ is odd} \end{cases} \tag{34}$$

and a normalization condition,

$$b_{N+J}(0) = 1.$$

In Appendix B it is shown how the complementary multipoint Padé approximant $B^c_{N(Q)+J}(x)$, which uses the same set of information together with the number E_{10},

is similarly defined. The main difference between the two approximants, aside from their complementary character and the occurrence of a pole located at $x = -E_{10}^2$, is that $B^c_{N(Q)+J}(x)$ agrees with $B(x)$ through the term in $(1/x)^J$ when $N + J$ is *odd* and through the term in $(1/x)^{J-1}$ is *even*. Thus, one of the two approximants $B_{N(Q)+J}(x)$ and $B^c_{N(Q)+J}(x)$ does not use all of the given information Eq. (31). The reason for this occurrence is that it is implicit in Eq. (31) that $B(x) \to 0$ as $x \to \infty$, and hence both approximants must do this also. Thus, in order that these two approximants be in the form of multipoint Padé approximants, the degree of the polynomial in denominator of each approximant must be exactly one greater than the degree of the polynomial in the numerator, and hence one of the approximants possesses insufficient parameters to allow it to match all of the given information.

To establish the existence and bounding properties of $B_{N(Q)+J}(x)$ we consider first the case $N = Q$ and use similar methods to those of Sec. 2.

As before, we make the decomposition (6) and set up the variational lower bound (7). The only difference here is that instead of using the trial function (11) we use

$$\sum_{r=1}^{[(Q+J)/2]} a_r (H_0 - E_0)^{2r-2} \left(\prod_{p=1}^{Q} [(H_0 - E_0)^2 + x_p]^{-1} \right) \sqrt{b},$$

where the a's are again the variational parameters. This trial function differs from (11) in that higher powers of $(H_0 - E_0)^2$ are included, thereby increasing the variational freedom of the trial function, and, as we shall see, these higher powers lead to the utilization of the additional information (31). In fact, the resulting functional can still be written in the form (12), except that the summations run up to $[(Q + J)/2]$ rather than $[Q/2]$, and we have

$$c_{rs}(x) = \sum_{p=1}^{Q} (-x_p)^{r+s-2} \left(\prod_{q=1}^{Q}{}' (x_q - x_p)^{-1} \right) \Big((x - x_p) B(x_p) + (x - x_p) \sum_{m=0}^{r+s-Q-2} (-x_p)^{-m-1} S(2m) + (-x_p)^{Q+1-r-s} S(2r + 2s - 2Q - 2) \Big)$$

for $r + s > Q$, and

$$d_r = \sum_{p=1}^{Q} (-x_p)^{r-1} \left(\prod_{q=1}^{Q}{}' (x_q - x_p)^{-1} \right) \left(\sum_{m=0}^{r-Q-1} (-x_p)^{-m-1} \times S(2m) - B(x_p) \right) \text{ for } r > Q.$$

The corresponding expressions when $r + s \leq Q$ and when $r \leq Q$, respectively, are given correctly in Eq. (12). It is thus seen that our new functional involves only the given information (1) and (31). In the case that $Q + J$ is odd no use is made of $S(2J - 2)$, as was discussed earlier.

The reasoning follows parallel lines to that given in Sec. 2. In place of Eq. (13) we obtain the lower bound

$$\gamma(x) \geq \hat{\gamma}_J(x) = \frac{\text{polynomial in } x \text{ of degree } [\frac{1}{2}(Q + J)] - 1}{\text{polynomial in } x \text{ of degree } [\frac{1}{2}(Q + J)]} = \frac{R([\frac{1}{2}(Q + J)] - 1; x)}{S([\frac{1}{2}(Q + J)]; x)}$$

The corresponding approximant to $B(x)$ is denoted by $\hat{B}_J(x)$, and it is obtained exactly as in Eq. (9);

$$\hat{B}_J(x) = \beta(Q - 1; x) + \left(\prod_{p=1}^{Q} (x_p - x) \right) \hat{\gamma}_J(x) = \frac{\beta(Q - 1; x) S([\frac{1}{2}(Q + J)]; x) + \left[\prod_{p=1}^{Q} (x_p - x) \right] R([\frac{1}{2}(Q + J)] - 1; x)}{S([\frac{1}{2}(Q + J)]; x)}. \quad (35)$$

The bounding properties of this approximant must be exactly the same as those tabulated in Eq. (10) for $\tilde{B}(x)$. We now show that $\hat{B}_J(x)$ is in fact the approximant defined by Eqs. (32), (33), and (34), in the case $Q = N$.

First we note that it is easily shown, by using an argument similar to the one given in Sec. 2, that $\prod_{p=1}^{Q} (x_p - x)$ can have no factors in common with $S([\frac{1}{2}(Q + J)]; x)$, whence

$$\hat{B}_J(x_p) = B(x_p) \quad \text{for} \quad p = 1, 2, \ldots, Q.$$

Again, following the argument given near the end of Sec. 2, we find here that

$$B(x) - \hat{B}_J(x) = \left(\prod_{p=1}^{Q} (x_p - x) \right) [\gamma(x) - \hat{\gamma}_J(x)] = O\left(\left(\frac{1}{x} \right)^{2[(Q+J)/2]+1-Q} \right).$$

In particular, the expansion of $B_J(x)$ in inverse powers of x agrees with Eq. (31) through the term in $(1/x)^J$ or $(1/x)^{J-1}$, according as $Q + J$ is even or odd, respectively. We are thus assured that the degree of the polynomial in the numerator of Eq. (35) is exactly $[\frac{1}{2}(P + J)] - 1$ and that $B_J(x)$ satisfies Eqs. (33) and (34) in the case $Q = N$. We conclude that $\hat{B}_J(x) \equiv B_{Q(Q)+J}(x)$.

The derivation can now be extended to establish the existence and bounding properties of $B_{N(Q)+J}(x)$ in the case $N > Q$. This can be done either by using the limiting argument given in Sec. 2 or, rigorously, by generalizing the variational derivation given in Appendix A.

It is found that the directions of the bounds supplied by $B_{N(Q)+J}(x)$ are exactly the same as those given by the $B_{N(Q)}(x)$ which uses only the given information (1). However, the bounds themselves are tighter because the inclusion of the additional information (31) has allowed the trial function Φ to have a greater variational freedom.

In Appendix B, we discuss briefly the complementary multipoint Padé approximant $B^c_{N(Q)+J}(x)$. This approximant yields bounds which are the exact complement to those which are supplied by the corresponding $B_{N(Q)+J}(x)$, together with the bound $B^c_{N(Q)+J}(x) \leq B(x)$ for $-E_{20}^2 < x < -E_{10}^2$. In fact the bounds are in the same direction as those given by the $B^c_{N(Q)}(x)$ which uses the same information (1), but no information of the form (31). Once again, however, the bounds are tighter.

As in previous cases we remark that to obtain these approximants in practice one should solve the set of defining equations directly, rather than following the variational procedure described here.

In the particular case that all of the information (1) is associated with the single point $x = 0$, the corresponding

$B_{N(1)+J}(x)$ becomes the "two-point" Padé approximant used by Tang[13] to bound the polarizability at imaginary frequencies.

Recently, Starkschall and Gordon[11] used a moment theoretical approach to obtain tight bounds on the van der Waals force constants for various atom–atom interactions. Their method can easily be shown to be equivalent to the use of the two multipoint Padé approximants $B_{N(Q)+J}(x)$ and $B^{c}_{N(Q)+J}(x)$ to bound $B(x)$ for $0 < x < \infty$. We thus see the essential unity of their approach with the earlier method used by Langhoff and Karplus[22] which involved the usual one-point Padé approximants.

5. THE NONOPTIMAL MULTIPONT PADÉ APPROXIMANTS

The various multipoint Padé approximants and their complements, as discussed in the foregoing sections, are clearly *variationally* optimal approximants. However, they can also be characterized as *physically* optimal. That this is so follows immediately from the following description of these approximants. Any one of these approximants can always be written in the form

$$V_0 + \sum_{n=1}^{m} \frac{c_{0n}}{(\hat{E}^2_{n0} + x)} \tag{36}$$

where $V_0 \geq 0$; $c_{0n} > 0$ $(n = 1, 2, \ldots, m)$ and the $\hat{E}_{n0}$ are variational upper bounds to the true excitation energies of the system as described earlier. For example, if the given information takes the form (1) with $N = Q$, then we have from Eqs. (20) and (14) that

$$B_{Q(Q)}(x) = \beta(Q-1;x) + \left(\prod_{p=1}^{Q}(x_p - x)\right) \sum_{n=1}^{[Q/2]} \frac{d_{0n}}{(\hat{E}^2_{n0} + x)},$$

where $d_{0n} > 0$ for $n = 1, 2, \ldots, [Q/2]$. Hence, using

$$B_{Q(Q)}(x) = \frac{\text{polynomial in } x \text{ of degree } [(Q-1)/2]}{\text{polynomial in } x \text{ of degree } [Q/2]}$$

and the result that

$$\lim_{x\to\infty} B_{Q(Q)}(x) \begin{cases} = 0 \text{ if } Q \text{ is even} \\ > 0 \text{ if } Q \text{ is odd} \end{cases},$$

we see that $B_{Q(Q)}(x)$ can indeed by written in the form (36), now with $m = [Q/2]$ and $V_0 = \lim B_{Q(Q)}(x)$ as $x \to \infty$.

Similar reasoning can be used in all other cases and the form (36) is readily verified in general. We now observe that (36) is itself essentially a polarizability function. If $V_0 = 0$ then (36) is the polarizability for a system whose oscillator strengths are precisely $c_{01}, c_{02}, \ldots, c_{0m}$ corresponding to energies $\hat{E}_{10}, \ldots, \hat{E}_{m0}$. If $V_0 > 0$ then we need only note that for finite x,

$$\lim_{E\to\infty}[V_0 E^2/(E^2 + x)] = V_0.$$

so that the V_0 term also corresponds to an oscillator strength and associated excitation energy, V_0E^2 and E, respectively, in the limit as $E \to \infty$. Thus, since these approximants are themselves essentially of the correct functional form and since any one approximant "matches" the information used to construct it, we conclude that these approximants are optimal in the sense described above.

The *nonoptimal* multipoint Padé approximants, although still displaying rigorous bounding properties, do not make such a best possible usage of the given information. However, they have the advantage that they are simpler to construct, and are anyway of interest in connection with the approximation of functions other than those which can be represented by a series of Stieltjes.[23]

We consider the case where the given information takes the form (1). The nonoptimal approximants considered here may then be defined as

$$B^{k}_{N(Q)}(x) = a^{k}_{N}(x)/b^{k}_{N}(x), \qquad 1 \leq k \leq [N/2], \tag{37}$$

where $a^{k}_{N}(x)$ and $b^{k}_{N}(x)$ are the polynomials of degrees $[(N-1)/2] + k$ and $[N/2] - k$, respectively, which are uniquely specified by the set of conditions

$$(B^{k}_{N(Q)})^{(n)}(x_p) = B^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases} \tag{38}$$

together with a normalization requirement,

$$b^{k}_{N}(0) = 1.$$

A similar definition can clearly be made for the closely related nonoptimal *complementary* multipoint Padé approximants. We will not discuss these here because the proof of their existence and bounding properties should become clear from the following derivation.

We will establish the existence and bounding properties of $B^{k}_{N(Q)}(x)$ by using a slight modification of the procedure used in Sec. 2.

Taking $Q = N$, we make the decomposition (6) and set up the variational lower bound $\tilde{\gamma}(x)$ to $\gamma(x)$, as in Eq. (7). In place of the trial function (11), we now use

$$\tilde{\Phi} = \begin{cases} \sum_{r=1}^{[Q/2]-k} a_r (H_0 - E_0)^{2r-2} \left(\prod_{p=1}^{Q} [(H_0 - E_0)^2 + x_p]^{-1}\right) \sqrt{b} \\ 0 \text{ if } k = [Q/2] \qquad\qquad \text{if } 1 \leq k < [Q/2] \end{cases}$$

which differs from Eq. (11) in having fewer terms.[24] On optimization of the corresponding functional, we obtain in place of Eq. (13);

$$\hat{\gamma}^{k}(x) = \begin{cases} \dfrac{\text{polynomial in } x \text{ of degree } [Q/2] - k - 1}{\text{polynomial in } x \text{ of degree } [Q/2] - k} \\ 0 \quad \text{if} \quad k = [Q/2] \end{cases}$$

$$= \frac{R([Q/2] - k - 1; x)}{S([Q/2] - k; x)}$$

where, as before, the coefficients involve only the given information. We now obtain an approximant $\hat{B}^{k}(x)$ to $B(x)$, just as was done in Eq. (14):

$$\hat{B}^{k}(x) = \beta(Q-1;x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)\hat{\gamma}^{k}(x) = \begin{cases} \dfrac{\beta(Q-1;x)S([Q/2]-k;x) + \left(\prod_{p=1}^{Q}(x_p - x)\right)R([Q/2]-k-1;x)}{S([Q/2]-k;x)} \\ \beta(Q-1;x) \quad \text{if} \quad k = [Q/2] \end{cases} \tag{39}$$

The bounding properties of the approximant must be exactly the same as those tabulated in Eq. (10) for $\tilde{B}(x)$. That is, the *directions* of the bounds supplied by $\hat{B}^k(x)$ with respect to $B(x)$ are exactly the same as those given by $B_{Q(Q)}(x)$. As before, it is easily shown that $S([Q/2] - k; x)$ can have no factors in common with $\prod_{p=1}^{Q}(x_p - x)$, and hence

$$\hat{B}^k(x_p) = B(x_p) \quad \text{for} \quad p = 1, 2, \ldots, Q.$$

Furthermore, it is not hard to prove using an argument similar to that in Sec. 2 that the degree of the polynomial in the numerator of Eq. (39) is in fact $[\frac{1}{2}(Q-1)] + k$. We conclude that $\hat{B}^k(x) \equiv B^k_{Q(Q)}(x)$ as defined by Eqs. (37) and (38), in the case $N = Q$.

To prove the existence and bounding properties of $B^k_{N(Q)}(x)$ when $N > Q$, one can either use the limiting argument of Sec. 2 or else make the obvious extension of the variational proof in Appendix A.

Although the directions of the bounds imposed by $B^k_{N(Q)}(x)$ on $B(x)$ are exactly the same as those of $B_{N(Q)}(x)$, the difference $|B(x) - B^k_{N(Q)}(x)|$ increases with increasing k due to the corresponding decrease in the variational freedom of the trial function. Thus, for example, one has

$$B^{[Q/2]}_{N(Q)}(Q) \leq B^{[Q/2]-1}_{N(Q)}(x) \leq \cdots \leq B^1_{N(Q)}(x) \leq B_{N(Q)}(x) \leq B(x) \quad \text{for} - E_{10}^2 < x < x_1.$$

In the particular case that all of the given information is associated with the single point $x = 0$, $B^k_{N(1)}(x)$ becomes the well-known $[[(N-1)/2] - k, [N/2] + k]$ one-point Padé approximant, and the usual inequalities[7] on these approximants are immediate.

ACKNOWLEDGMENTS

S.T.E. wishes to thank Professor C. A. Coulson for making his stay in Oxford such a pleasant one.

APPENDIX A: VARIATIONAL PROOF OF THE EXISTENCE AND BOUNDING PROPERTIES OF $B_{N(Q)}(x)$ IN THE GENERAL CASE $N \geq Q$

We are given the set of N pieces of information (1) about $B(x)$, and we wish to establish directly both the existence and bounding properties of the corresponding multipoint Padé approximant $B_{N(Q)}(x)$ as defined in Eqs. (17) and (18).

To this end we write, in place of Eq. (16),

$$B(x) = \beta(N-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)^{N_p}\right)\gamma(x), \tag{A1}$$

where now $\beta(N-1; x)$ is the unique polynomial of degree $N-1$ which satisfies

$$\beta^{(n)}(N-1; x_p) = B^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases}$$

and where

$$\gamma(x) = \sum_n{}' \frac{b_{0n}}{(E_{n0}^2 + x_1)^{N_1}(E_{n0}^2 + x_2)^{N_2}\cdots(E_{n0}^2 + x_Q)^{N_Q}(E_{n0}^2 + x)} = \left(\sqrt{b}, \left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-N_p}\right)[(H_0 - E_0)^2 + x]^{-1}\sqrt{b}\right). \tag{A2}$$

This algebraic identity is easily proved by using induction. If now we introduce the functional

$$\tilde{\gamma}(x) = -\left(\tilde{\Phi}, \left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{N_p}\right)[(H_0 - E_0)^2 + x]\right) + (\tilde{\Phi}, \sqrt{b}) + (\sqrt{b}, \tilde{\Phi}),$$

then it is not hard to show that

$$\tilde{\gamma}(x) \leq \gamma(x) \quad \text{for} \quad -E_{10}^2 < x < \infty$$

providing that the trial function $\tilde{\Phi}$ satisfies

$$(\tilde{\Phi}, \psi_0) = 0.$$

Suppose that we have any such lower bound $\tilde{\gamma}(x)$ to $\gamma(x)$. On substitution into Eq. (A1) we obtain an approximant for $B(x)$,

$$\tilde{B}(x) = \beta(N-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)^{N_p}\right)\tilde{\gamma}(x)$$

whose bounding properties are readily verified to be those tabulated for $B_{N(Q)}(x)$ in Eq. (22). That is, they are exactly the same as would be obtained if one had started with the set of bounds (10) and then followed the limiting process described near the end of Sec. 2.

If we now use the trial function

$$\tilde{\Phi} = \sum_{r=1}^{[N/2]} a_r (H_0 - E_0)^{2r-2}\left(\prod_{p=1}^{Q}[(H_0 - E_0)^2 + x_p]^{-N_p}\right)\sqrt{b}$$

in Eq. (A2) and optimize the variational parameters $a_1, a_2, \ldots, a_{[N/2]}$, we obtain the lower bound to $\gamma(x)$:

$$\hat{\gamma}(x) = \frac{\text{polynomial in } x \text{ of degree } [N/2] - 1}{\text{polynomial in } x \text{ of degree } [N/2]} = \frac{R[N/2] - 1; x)}{S[N/2/; x)}$$

where the coefficients can be shown to involve only the given information (1).

The corresponding approximant to $B(x)$ is

$$\hat{B}(x) = \beta(N-1; x) + \left(\prod_{p=1}^{Q}(x_p - x)^{N_p}\right)\hat{\gamma}(x),$$

and similar arguments to those used in Sec. 2 suffice to ensure that this approximant is precisely $B_{N(Q)}(x)$ defined by Eqs. (17) and (18).

APPENDIX B: THE COMPLEMENTARY MULTIPOINT PADÉ APPROXIMANT $B^c_{N(Q)+J}(x)$

Suppose we are given the sets of information (1) and (31), and the number E_{10}, all pertaining to $B(x)$. Then the complementary multipoint Padé approximant $B^c_{N(Q)+J}(x)$ which corresponds to this information is defined by

$$B^c_{N(Q)+J}(x) = c_{N+J}(x)/d_{N+J}(x)$$

where $c_{N+J}(x)$ and $d_{N+J}(x)$ are the polynomials of degrees $[\frac{1}{2}(N+J+1)] - 1$ and $[\frac{1}{2}(N+J+1)]$, respectively, which are uniquely specified by the requirements

$$(B^{c}_{N(Q)+J})^{(n)}(x_p) = B^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases},$$

$$B^{c}_{N(Q)+J}(x) \sim S(0)(1/x) - S(2)(1/x)^2 + \cdots +$$

$$+ \begin{cases} (-1)^{J+1} S(2J-2)(1/x)^J & \text{if } N+J \text{ is odd} \\ (-1)^J S(2J-4)(1/x)^{J-1} & \text{if } N+J \text{ is even} \end{cases}$$

together with the two conditions

$$d_{N+J}(0) = 1 \quad \text{and} \quad d_{N+J}(-E_{10}^2) = 0.$$

The proof of the existence and bounding properties of this approximant (which are described in Sec. 4), rests on Sec. 3 in the same way as the proof relating to $B_{N(Q)+J}(x)$ rests on Sec. 2.

APPENDIX C: MULTIPOINT PADE APPROXIMANTS FOR ARBITRARY FUNCTIONS WHICH CAN BE REPRESENTED BY A SERIES OF STIELTJES

If $S(x)$ is a function which can be represented by a series of Stieltjes with radius of convergence R, then it can be written in the form

$$S(x) = \int_0^{1/R} \frac{d\phi(u)}{(1+ux)}, \tag{C1}$$

where $\phi(u)$ is a bounded, monotone nondecreasing function, which attains infinitely many different values for $0 \leq u \leq 1/R$.

We can rewrite Eq. (C1) as

$$S(x) = \int_R^{\infty} \frac{v d\eta(v)}{(v+x)} + c, \tag{C2}$$

where $\eta(v)$ is sufficiently defined by the condition

$$d\eta(v) = -d\phi(1/v), \qquad R \leq v < \infty,$$

and c is the nonnegative constant given by

$$c = \lim_{u \to 0+} [\phi(u) - \phi(0)].$$

We notice that $\eta(v)$ is also a bounded, monotone nondecreasing function, except that now the infinitely many different values are attained for $R \leq v < \infty$, and hence the integral in Eq. (C2) exists in the Riemann–Stieltjes sense for $-R < x \leq \infty$. In fact $S(x)$ is a continuous monotone decreasing function over this interval, tending to the value $c \geq 0$ as $x \to \infty$. Our objective here is to write $\tilde{S}(x) = S(x) - c$ in the *form* of a dynamical polarizability $B(x)$. This having been achieved we will show how the variational formulation in the body of the paper can be generalized so that it applies to $\tilde{S}(x)$. It is then an easy matter to establish the existence and bounding properties of the various multipoint Padé approximants for $S(x)$ itself.

To this end we now rewrite Eq. (C2) as

$$\tilde{S}(x) = S(x) - c = \int_{R^{1/2}}^{\infty} \frac{\epsilon d\xi(\epsilon)}{(\epsilon^2 + x)}, \tag{C3}$$

where $\xi(\epsilon)$ is defined by

$$d\xi(\epsilon) = \epsilon d\eta(\epsilon^2), \qquad R^{1/2} \leq \epsilon < \infty.$$

Here we note that although $\xi(\epsilon)$ is not necessarily bounded, the funtion $\Xi(\epsilon) = \int_{R^{1/2}}^{\epsilon} d\xi(\epsilon)/\epsilon$ *is* bounded, being also monotone nondecreasing and attaining infinitely many different values for $R^{1/2} \leq \epsilon < \infty$, and hence the integral in Eq. (C3) is well defined for $R < x < \infty$.

The function $\tilde{S}(x)$ is now seen to be of the same form as the dynamical polarizability $B(x)$ defined in Eq. (2). In fact, $S(x)$ *is* the polarizability for an artificial system whose excitation energies are exactly the points of increase of $\xi(\epsilon)$, and whose cumulative oscillator strength function $F(\epsilon)$ is given by[25]

$$F(\epsilon) = \int_{R^{1/2}}^{\epsilon} \epsilon' \, d\xi(\epsilon').$$

To make this connection between $\tilde{S}(x)$ and the dynamical polarizability more formal, we proceed as follows. Let $\mathcal{E}$ denote the set of real numbers

$$\mathcal{E} = \{0\} \cup \{\epsilon \in [R^{1/2}, \infty) : d\xi(\epsilon)/d\epsilon \neq 0\},$$

and let $\tilde{H}_0$ be a Hermitian operator with lowest eigenvalue $\tilde{E}_0$, such that the eigenvalue spectrum of $(\tilde{H}_0 - \tilde{E}_0)$ is precisely the set $\mathcal{E}$. Let $\{\tilde{\psi}_\epsilon\}_{\epsilon \in \mathcal{E}}$ denote the normalized eigenvectors of $(\tilde{H}_0 - \tilde{E}_0)$, so that $(\tilde{H}_0 - \tilde{E}_0)\tilde{\psi}_0 = 0$, and denote the corresponding Hilbert space by $\mathcal{H}$. Now take $\tilde{V}$ to be any self-adjoint operator over $\mathcal{H}$ such that[25]

$$\tilde{V}\tilde{\psi}_0 = \sum_{\epsilon \in \mathcal{E}}{}' [d\xi(\epsilon)/d\epsilon]^{1/2} \tilde{\psi}_\epsilon,$$

where the summation is understood to include integration over all continuous regions in $\mathcal{E}$.

It is now easy to see that we can rewrite

$$\tilde{S}(x) = \sum_{\epsilon}{}' \frac{\tilde{b}_{0\epsilon}}{(\tilde{E}^2_{\epsilon 0} + x)}, \tag{C4}$$

where $\tilde{E}_{\epsilon 0} = \epsilon$ is the "excitation energy" for a transition from the state $\tilde{\psi}_0$ to the state $\tilde{\psi}_\epsilon$, and $\tilde{b}_{0\epsilon}$ is the corresponding "oscillator strength"

$$\tilde{b}_{0\epsilon} = \tilde{E}_{\epsilon 0}(\tilde{\psi}_0, \tilde{V}\tilde{\psi}_\epsilon)(\tilde{\psi}_\epsilon, \tilde{V}\tilde{\psi}_0).$$

Comparison of Eq. (C4) with Eq. (2) leads us to conclude that any function which can both be represented by a series of Stieltjes, and which tends to zero as $x \to \infty$, can also be described as a dynamical polarizability for an artificial physical system, indicated by a Hamiltonian $\tilde{H}_0$ and a self-adjoint perturbation $\tilde{V}$.

Thus, replacing $(H_0 - E_0)$ by $(\tilde{H}_0 - \tilde{E}_0)$, ψ_n by $\tilde{\psi}_n$, b_{0n} by $\tilde{b}_{0n}$, and so on, throughout the main text of this paper, we see that we have achieved a variational proof for the existence and bounding properties of the various multipoint Padé approximants to $\tilde{S}(x)$. For example, we are now assured of the existence of the approximant $\tilde{S}_{N(Q)}(x)$ to $\tilde{S}(x)$ defined by

$$\tilde{S}_{N(Q)}(x) = a_N(x)/b_N(x),$$

where $a_N(x)$ and $b_N(x)$ are the polynomials of degrees $[(N-1)/2]$ and $[N/2]$, respectively, which are uniquely specified by the set of conditions

$$\tilde{S}^{(n)}_{N(Q)}(x_p) = \tilde{S}^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases}$$

and

$$b_N(0) = 1,$$

where

$$-R < x_1 < x_2 < \cdots < x_Q < \infty \quad \text{and} \quad \sum_{p=1}^{Q} N_p = N.$$

Further, we have established that $\bar{S}_{N(Q)}(x)$ imposes rigorous bounds on $\bar{S}(x)$ which are the same as those tabulated in Eq. (22) for $B_{N(Q)}(x)$ with respect to $B(x)$.

We now wish to demonstrate that the added constant c, which relates $\bar{S}(x)$ to arbitrary functions representable by a series of Stieltjes, makes no difference to the existence and bounding properties of the corresponding multipoint Padé approximants. We will consider the cases N odd and N even separately. The given information pertains now to $S(x)$, and for simplicity we will suppose that it is of type (1).

N odd: Suppose for the moment that we know the constant c. Then by using the relation $S(x) = \bar{S}(x) + c$ we can transform the given information about $S(x)$ into a corresponding set of information about $\bar{S}(x)$. We can now construct the approximant $\bar{S}_{N(Q)}(x)$ to $\bar{S}(x)$, whose existence and bounding properties have already been established. Now consider the function

$$T_{N(Q)}(x) = \bar{S}_{N(Q)}(x) + c.$$

It is easily seen that, because N is odd, this can be written as

$$T_{N(Q)}(x) = \frac{\text{polynomial in } x \text{ of degree } [(N-1)/2]}{\text{polynomial in } x \text{ in degree } [N/2]}$$

and, furthermore, that it satisfies

$$T^{(n)}_{N(Q)}(x_p) = S^{(n)}(x_p) \quad \text{for} \begin{cases} n = 0, 1, \ldots, N_{p-1} \\ p = 1, 2, \ldots, Q \end{cases}.$$

But the latter two statements tell us that we have, in fact, constructed $S_{N(Q)}(x) \equiv T_{N(Q)}(x)$ because of the uniqueness of the approximant, and, hence, $S_{N(Q)}(x)$ can be constructed directly without invoking the constant c. The relationship between $\bar{S}_{N(Q)}(x)$ and $S_{N(Q)}(x)$ tells us that the bounding properties of $S_{N(Q)}(x)$ with respect to $S(x)$ are exactly the same as those of $\bar{S}_{N(Q)}(x)$ with respect to $\bar{S}(x)$ i.e., identical with those tabulated in Eq. (22) for $B_{N(Q)}(x)$ with respect to $B(x)$.

N even: Here we appeal to the well-known result[21] that if $S(x)$ is representable by a series of Stieltjes with radius of convergence R, then

$$U(x) = [S(x_1) - S(x)]/(x - x_1)S(x) \qquad \text{(C5)}$$

is also representable by a series of Stieltjes, but with radius of convergence at least R.

Hence, if we are given a set of N pieces of information of type (1) about $S(x)$, we can use Eq. (C5) to transform this set into $(N-1)$ pieces of information about $U(x)$. Since $(N-1)$ is an odd integer, we are assured of the existence of the corresponding approximant $U_{(N-1)(Q)}(x)$ to $U(x)$, say. The desired approximant to $S(x)$ is easily seen to be

$$S_{N(Q)}(x) = S(x_1)/[1 + (x - x_1)U_{(N-1)(Q)}(x)],$$

and using the known bounding relationship between $U(x)$ and $U_{(N-1)Q}(x)$, it is readily verified that the bounding properties of $S_{N(Q)}(x)$ with respect to $S(x)$ are again the same as those tabulated in Eq. (22).

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*Work done while a Guggenheim Fellow at the Mathematical Institute, Oxford, England; on leave from the University of Wisconsin.
†This work was supported by the National Science Foundation Grant GP-28213.

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[17] M. Karplus and H. J. Kolker, J. Chem. Phys. 41, 3955 (1964).
[18] The trial function $\tilde{\theta} = \Sigma_{r=0}^{[Q/2]-1} a_r\theta_r$ (in obvious notation) is such that it could be accurate through the term in $(1/x)^{[Q/2]-1}$. The corresponding optimization condition reads $\Sigma_{s=0}^{[Q/2]-1} \hat{a}_s(\theta_r, (1+[H_0 - E_0]^2(1/x))\theta_s) = (\theta_r, W^{1/2}\sqrt{b})$ $(r=0,1,\ldots,[Q/2]-1)$. This set of equations is clearly equivalent to the set one obtains on projecting the exact equation $[1+[H_0 - E_0]^2(1/x)]\theta = W^{1/2}\sqrt{b}$ [Eq.(*)] onto the space spanned by $\theta_0, \theta_1, \ldots, \theta_{[Q/2]-1}$. Since this projection cannot alter the solution to (*) through the term in $(1/x)^{[Q/2]-1}$ we conclude that $\tilde{\theta} = \Sigma_{r=0}^{[Q/2]-1} a_r\theta_r$ must indeed be accurate through the term in $(1/x)^{[Q/2]-1}$.

[19] The set of Eqs.(18) can be linearized to read $a_N^{(n)}(x_p) - \Sigma_{m=1}^{n} \binom{n}{m} B^{(n)}(x_p) b_N^{(n-m)}(x_p) = 0$ $(n = 0, 1, \ldots, N_{p-1}; p = 1, 2, \ldots, Q)$. Together with the normalization condition $b_N(0) = 1$, these equations constitute $N+1$ linear equations in $N+1$ unknowns.
[20] It is also possible to use a lower bound E_{10}^L to E_{10}. The bounding properties of the resulting approximant are much the same as those described later in this section, except that now one has only an upper bound for $-E_{10}^{L^2} < x < x_1$, rather than the bounds $B^c_{N(Q)}(x) \leqslant B(x)$ for $-E_{20}^2 < x < -E_{10}^2$ and $B^c_{N(Q)}(x) \geqslant B(x)$ for $-E_{10}^2 < x < x_1$.
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[23] For example, a nonoptimal Padé approximant would be better than an optimal Padé approximant if the function to be approximated is of the form $P(x) + S(x)$, where $P(x)$ is a polynomial of finite degree and $S(x)$ is representable by a series of Stieltjes.
[24] Here one could make many other choices for the trial function $\tilde{\Phi}$ such that only the given information would be utilized in the resulting approximants. For example, one could take the range of summation to be $\Sigma_{r=k+1}^{[Q/2]}$ rather than $\Sigma_{r=1}^{[Q/2]-k}$. In this way one can generate whole families of rational approximations to $B(x)$, each member of which matches $B(x)$ at the data points and which imposes rigorous bounds on $B(x)$ elsewhere for $-E_{10}^2 < x < \infty$.

[25] It is clearly possible that $F(\epsilon) \to \infty$ as $\epsilon \to \infty$. Correspondingly we then have $|\tilde{V}\psi_0| = \infty$, and the formal use of such a $\tilde{V}$ in the variational formulation given in the body of the paper might then be considered unrigorous. However, this objection can be circumvented as follows. Instead of starting with the representation (C3), we could have proceeded directly from (C1), writing $\tilde{S}(x) = \int_{0^+}^{1/R} [d\phi(u)/(1 + ux)]$. If we then choose an H whose spectrum is the points of increase of $\phi(u)$ in $(0, 1/R)$ together with the number 0, so that $H\psi_0 = 0$, then we can define a self-adjoint operator W such that $W\psi_0 = \Sigma_\epsilon^1 [d\phi(\epsilon)/d\epsilon]^{1/2}\psi_\epsilon$. We then have $S(x) = (\psi_0, W(1 + Hx)W\psi_0)$, and a variational lower bound is, for example, $(x) = -(\Phi, (1 + Hx)\Phi) + 2(\Phi, W\psi_0)$. The operator W can clearly be chosen so that it is bounded, and the derivation can be carried through in a manner similar to that used in the paper.

Solution of the Hamilton–Jacobi equation for certain dissipative classical mechanical systems

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(Received 16 August 1972)

Recent developments have shown that the pure Lagrange–Hamiltonian formalisms can be extended to problems (chiefly, classical systems involving dissipative forces) previously regarded as outside such theories. The Hamilton–Jacobi equations corresponding to certain such systems are given here, and the structure, separability, and solution of these equations are studied. Examples treated here include a particle moving freely and under a constant force in a viscous medium, the damped-harmonic oscillator in one and three dimensions, and a particle moving in one dimension with quadratic friction in an arbitrary potential. In all cases, the Hamilton–Jacobi equation separates into time and space components, and the complete solution is obtained.

1. INTRODUCTION

The time evolution of a classical mechanical system can be described in four ways. First, one can identify the forces acting on the system, and write the equations of motion from Newton's laws. Second, one may be able to construct a Lagrangian $L(\dot{q}_i, q_i, t)$ which has the equations of motion as its Euler–Lagrange equations following from Hamilton's principle. Third, one may find a Hamiltonian function $H(p_i, q_i, t)$ of the canonical coordinates q_i and momenta p_i such that Hamilton's dynamical equations correspond to the equations of motion. Lastly, if such a Hamiltonian exists, one can instead construct the Hamilton–Jacobi partial differential equation, and obtain the motion of the system from it.

For conservative systems, the above procedures are reasonably straightforward, since one then knows the structures of $L(L = T - V)$ and $H(H = T + V)$, where T is the kinetic and V the potential energy. Then H is a constant of the motion which we call the total energy E, and the Hamilton–Jacobi equation

$$H(\partial\phi/\partial q_i, q_i) + \partial\phi/\partial t = 0 \tag{1.1}$$

permits the separation of ϕ into spacial and temporal parts

$$\phi(q_i, \alpha_i, t) = S(q_i, \alpha_i) - Et, \tag{1.2}$$

where the α_i are parameters (E and the α_i are not independent).

However, for dissipative systems, it had been thought only the first procedure above was applicable, as neither separable Lagrangian[1] nor Hamiltonian[2] functions existed for such systems. (Frictional forces can be *added* to Lagrange's or Hamilton's equation, as has been done via the Rayleigh dissipative function,[3] but such an ad hoc procedure destroys the essence of the Lagrangian and Hamiltonian methods, and therefore should be avoided.) Recently,[4] pure Lagrangian descriptions which yield dissipative forces have been found for certain systems. Since such Lagrangians imply the existence of Hamiltonians yielding the same equations of motion, it is of interest to examine the structure, separability and solution of the Hamilton–Jacobi equations generated in these cases, and to compare them with the conventional Hamilton–Jacobi equations for conservative systems.

Further, since classical Hamilton–Jacobi theory for conservative systems forms a link with quantum mechanics, it is of particular importance to examine these classical dissipative systems to see if they lead to a quantum mechanical treatment of dissipation. This will be discussed in a later paper.

2. ONE-DIMENSIONAL VISCOUS MEDIUM

A particle travelling in one dimension through a linearly viscous medium is characterized by the equation of motion (let the mass m be 1)

$$\ddot{x} + \gamma\dot{x} = 0. \tag{2.1}$$

A Lagrangian which generates (2.1) as its Euler–Lagrange equation is

$$L = \tfrac{1}{2}e^{\gamma t}\dot{x}^2, \tag{2.2}$$

and the corresponding Hamiltonian

$$H = \tfrac{1}{2}p^2e^{-\gamma t}, \tag{2.3}$$

where $p = \dot{x}e^{\gamma t}$ is the canonical momentum.

The Hamilton–Jacobi equation is then

$$\tfrac{1}{2}e^{-\gamma t}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{\partial\phi}{\partial t} = 0, \tag{2.4}$$

where $\phi = \phi(x, \alpha, t)$, α is a parameter, and $p = \partial\phi/\partial x$. The x and t variables are separated by the assumption

$$\phi = Q(x, \alpha)T(t), \tag{2.5}$$

from which one finds that $T = e^{\gamma t}$ is sufficient to accomplish the separation. (While other forms of T are possible, they introduce extraneous parameters.) Then (2.4) reduces to

$$(Q')^2 + 2\gamma Q = 0, \tag{2.6}$$

where $Q' = dQ/dx$. Thus,

$$Q = -\tfrac{1}{2}\gamma(x - c)^2. \tag{2.7}$$

Note that the dependence of Q on $x - c$ is expected from the x-translation invariance of (2.4).[5]

From the auxiliary condition $\beta = \partial\phi/\partial\alpha$, with the identification $\alpha \sim c$,

$$\beta = \gamma e^{\gamma t}(x - c), \tag{2.8}$$

from which

$$x = c + (\beta/\gamma)e^{-\gamma t}, \tag{2.9}$$

the solution of (2.1).

3. LINEARLY DAMPED PARTICLE WITH CONSTANT FORCE

The linearly damped particle moving in one dimension under a constant force has the equation of motion

$$\ddot{x} + \gamma\dot{x} + g = 0. \tag{3.1}$$

A suitable Lagrangian is

$$L = e^{\gamma t}(\tfrac{1}{2}\dot{x}^2 - gx), \tag{3.2}$$

and the corresponding Hamiltonian

$$H = \tfrac{1}{2}p^2e^{-\gamma t} + gxe^{\gamma t}. \tag{3.3}$$

The Hamilton–Jacobi equation is then

$$\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 e^{-\gamma t} + gxe^{\gamma t} + \frac{\partial\phi}{\partial t} = 0, \tag{3.4}$$

and the separation (2.5) gives

$$(Q')^2 + 2\gamma Q + 2gx = 0. \tag{3.5}$$

[As $p = \dot{x}e^{\gamma t}$, $Q' = \dot{x} = v$. Since v is real, $(Q')^2 \geq 0$, implying that $\gamma Q + gx \leq 0$.]

If (3.5) is differentiated with respect to x, and Q' is replaced by y, (3.5) becomes

$$yy' + \gamma y + g = 0, \tag{3.6}$$

which is separable, and integration yields the implicit relation

$$-[\gamma y + g - g\ln(\gamma y + g)] = \gamma^2(x + c). \tag{3.7}$$

Differentiating (3.7) with respect to c,

$$-\frac{1}{2}\frac{\partial y^2}{\partial c} = \gamma y + g. \tag{3.8}$$

From (3.5) and (3.8),

$$\gamma\frac{\partial Q}{\partial c} = \gamma y + g, \tag{3.9}$$

and (3.7) becomes

$$\gamma\frac{\partial Q}{\partial c} - g\ln\left(\gamma\frac{\partial Q}{\partial c}\right) = -\gamma^2(x + c). \tag{3.10}$$

Then, if the parameter α is identified as c,

$$\beta = \frac{\partial\phi}{\partial\alpha} = e^{\gamma t}\frac{\partial\phi}{\partial c}, \tag{3.11}$$

and (3.10) implies

$$x = (g/\gamma^2)\ln(\gamma\beta) - c - (\beta/\gamma)e^{-\gamma t} - (g/\gamma)t, \tag{3.12}$$

the solution to (3.1).

4. THE LINEARLY DAMPED HARMONIC OSCILLATOR

The linearly damped, one-dimensional harmonic oscillator is governed by the equation of motion

$$\ddot{x} + 2\gamma\dot{x} + \omega_0^2x = 0, \tag{4.1}$$

which is generated by the Lagrangian[4]

$$L = \tfrac{1}{2}e^{2\gamma t}(\dot{x}^2 - \omega_0^2x^2). \tag{4.2}$$

Then the canonical momentum p is

$$p = \dot{x}e^{2\gamma t}, \tag{4.3}$$

and the corresponding Hamiltonian

$$H = \tfrac{1}{2}(p^2e^{-2\gamma t} + \omega_0^2x^2e^{2\gamma t}). \tag{4.4}$$

The Hamilton–Jacobi equation is

$$\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 e^{-2\gamma t} + \tfrac{1}{2}\omega_0^2x^2e^{2\gamma t} + \frac{\partial\phi}{\partial t} = 0. \tag{4.5}$$

As in the previous sections, t and x are separated by

$$\phi = -e^{2\gamma t}Q(x, \alpha), \tag{4.6}$$

where Q satisfies

$$(Q')^2 + \omega_0^2x^2 - 4\gamma Q = 0. \tag{4.7}$$

To obtain the solution to (4.7), note that the transformations

$$Q \to a^2Q, \qquad x \to ax \tag{4.8}$$

leave the equation invariant. Such invariance implies the existence of a conserved quantity.[6] Consider the differential invariants

$$u = -Q'/x, \qquad xu' + u = -Q''. \tag{4.9}$$

After differentiation of (4.7) and substitution from (4.9), one obtains

$$xuu' + u^2 + 2\gamma u + \omega_0^2 = 0,$$

or

$$\frac{udu}{u^2 + 2\gamma u + \omega_0^2} = -\frac{dx}{x}. \tag{4.10}$$

Integrating, one gets

$$\ln[(u + \gamma)^2 + \omega^2] - (2\gamma/\omega)\tan^{-1}[(u + \gamma/\omega] + \ln x^2 = C, \tag{4.11}$$

where $\omega^2 = \omega_0^2 - \gamma^2$. Replacing u by v/x, one has

$$\ln[(v + \gamma x)^2 + \omega^2x^2] - (2\gamma/\omega)\tan^{-1}[(v + \gamma x)/\omega x] = C. \tag{4.12}$$

This constant C is identical to that obtained from the time-translation invariance of (4.1).[7] [Differentiation of (4.12) with respect to t of course yields the equation of motion.]

Another form of H in this case, as given by Havas,[4] is

$$H_h = -\gamma xp_h + \ln x - \ln(\cos\omega xp_h), \tag{4.13}$$

where p_h is not the canonical momentum in (4.3). Then

$$\dot{x} = v = -\gamma x + \omega x \tan\omega x p_h, \tag{4.14}$$

and H_h can be written

$$H_h = -(\gamma/\omega)\tan^{-1}[(v+\gamma x)/\omega x] - \ln\omega + \tfrac{1}{2}\ln[(v+\gamma x)^2 + \omega^2 x^2]. \tag{4.15}$$

Thus, $2(H_h + \ln\omega) = C$, so that the constant of the motion generated by the time-translation invariance of the equation of motion (or from the Hamilton–Jacobi equation) is equivalent to H_h. Or, time-translation invariance has generated a Hamiltonian, rather than *vice versa*. The Hamiltonians (4.4) and (4.13) must be q-equivalent, in the terminology of Currie and Saletan.[2]

Returning to the solution of the Hamilton–Jacobi equation, (4.7), (4.9) and (4.11) may be combined to express (implicitly) Q as a function of x and C. To obtain the motion, consider

$$\beta = \frac{\partial\phi}{\partial\alpha} = \frac{\partial\phi}{\partial C} = -e^{2\gamma t}\frac{\partial Q}{\partial C}, \tag{4.16}$$

where the parameter α is identified as C. Since Q cannot be written explicitly as $Q(x, C)$, implicit differentiation is employed.

Operating on (4.11) with $\partial/\partial C$,

$$\frac{\partial u^2}{\partial C} = (u+\gamma)^2 + \omega^2, \tag{4.17}$$

while, from (4.7) and (4.9),

$$u^2 = 4\gamma(Q/x^2) - \omega_0^2, \tag{4.18}$$

so that

$$\frac{\partial Q}{\partial C} = \frac{x^2}{4\gamma}[(u+\gamma)^2 + \omega^2]. \tag{4.19}$$

Thus, (4.11) becomes

$$\ln\left(4\gamma\frac{\partial Q}{\partial C}\right) - \frac{2\gamma}{\omega}\sec^{-1}\left[\frac{1}{\omega^2 x^2}\frac{4\gamma}{}\frac{\partial Q}{\partial C}\right]^{1/2} = C. \tag{4.20}$$

Let $\beta = -\lambda$ in (4.16), so that (4.20) becomes

$$\delta - \omega t = \sec^{-1}\left[\frac{(4\gamma\lambda)^{1/2}}{\omega} \quad \frac{e^{-\gamma t}}{x}\right],$$

where δ is a constant. Then

$$x = (4\gamma\lambda/\omega)^{1/2}e^{-\gamma t}\cos(\omega t - \delta),$$

the well-known solution for the damped harmonic oscillator.

The more general equation of motion

$$\ddot{x} + \gamma\dot{x} + f(x) = 0, \tag{4.21}$$

is generated by the Hamiltonian

$$H = \tfrac{1}{2}p^2 e^{-\gamma t} + e^{\gamma t}V(x), \tag{4.22}$$

where $V = \int f(x)dx$. The Hamilton–Jacobi equation is then

$$\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 e^{-\gamma t} + Ve^{\gamma t} + \frac{\partial\phi}{\partial t} = 0.$$

Separation of variables again obtains from $\phi = Q(x, \alpha)e^{\gamma t}$, from which

$$\tfrac{1}{2}(Q')^2 + V(x) = \gamma Q. \tag{4.23}$$

No general solution to (4.23) is known, but, since $Q' = v$, differentiation of (4.23) with respect to t yields the equation of motion (4.21).

5. LINEAR FRICTION IN THREE DIMENSIONS

For a particle moving in three-dimensional (Euclidean) space, with linear friction and under forces derivable from a scalar potential, the equation of motion is

$$\ddot{\mathbf{r}} + \gamma\dot{\mathbf{r}} = \mathbf{f} = -\nabla V(\mathbf{r}). \tag{5.1}$$

This equation is derivable from the Hamiltonian

$$H = \tfrac{1}{2}p^2 e^{-\gamma t} + V(\mathbf{r})e^{\gamma t}, \tag{5.2}$$

and the associated Hamilton–Jacobi equation is

$$\tfrac{1}{2}(\nabla\phi)^2 e^{-\gamma t} + Ve^{\gamma t} + \frac{\partial\phi}{\partial t} = 0. \tag{5.3}$$

Separation of space and time variables is again obtained from

$$\phi = W(\mathbf{r}, \boldsymbol{\alpha})e^{\gamma t},$$

and the spacial equation is

$$\tfrac{1}{2}(\nabla W)^2 + V + \gamma W = 0. \tag{5.4}$$

If $V(x, y, z) = V_1(x) + V_2(y) + V_3(z)$, then the separation

$$W = X(x, \alpha_1) + Y(y, \alpha_2) + Z(z, \alpha_3)$$

gives

$$\frac{1}{2}\left(\frac{dX}{dx}\right)^2 + V_1(x) + \gamma X = C_1, \tag{5.5a}$$

$$\frac{1}{2}\left(\frac{dY}{dy}\right)^2 + V_2(y) + \gamma Y = C_2, \tag{5.5b}$$

$$\frac{1}{2}\left(\frac{dZ}{dz}\right)^2 + V_3(z) + \gamma Z = C_3, \tag{5.5c}$$

where C_1, C_2, and C_3 are separation constants, and

$$C_1 + C_2 + C_3 = 0. \tag{5.6}$$

Setting

$$\bar{X}(x, \alpha_1) = X(x, \alpha_1) - C_1/\gamma, \quad \text{etc.}, \tag{5.7}$$

yields

$$\frac{1}{2}\left(\frac{d\bar{X}}{dx}\right)^2 + V_1(x) + \gamma\bar{X} = 0, \quad \text{etc.}, \tag{5.8}$$

and as

$$\phi = e^{\gamma t}[\bar{X} + (C_1/\gamma) + \bar{Y} + (C_2/\gamma) + \bar{Z} + (C_3/\gamma)], \tag{5.9}$$

with

$$\beta_1 = \frac{\partial\phi}{\partial\alpha_1} = e^{\gamma t}\frac{\partial\bar{X}}{\partial\alpha_1}, \quad \text{etc.}, \tag{5.10}$$

for $\alpha_1 \neq C_1$, etc., it is seen that there is no loss of generality in setting $C_1 = C_2 = C_3 = 0$. The solutions for the potentials treated in the previous sections thus follow.

6. QUADRATIC FRICTION

The equation of motion for the one-dimensional, quadratically damped particle is given by

$$\ddot{x} \pm c\dot{x}^2 + f(x) = 0, \tag{6.1}$$

where the $\pm$ sign is chosen so that the friction always opposes the motion. A piecewise-smooth Lagrangian generating (6.1) is given by[4,7]

$$L = \tfrac{1}{2}\dot{x}^2 e^{\pm 2cx} - \int e^{\pm 2cx} f(x)dx, \tag{6.2}$$

and the Hamiltonian is

$$H = \tfrac{1}{2} e^{\mp 2cx} p^2 + \int e^{\pm 2cx} f(x)dx, \tag{6.3}$$

a constant of the motion generated by the time-translation invariance of (6.1).[7]

With respect to Hamilton–Jacobi theory, since H is independent of t, this can be *treated* as a conservative system, so that

$$H\left(x, \frac{\partial \phi}{\partial x}\right) + \frac{\partial \phi}{\partial t} = 0,$$

and separation of variables results from setting

$$\phi(x, \alpha, t) = S(x, \alpha) - Et.$$

Thus,

$$\tfrac{1}{2}(S')^2 e^{\mp 2cx} + \int e^{\mp 2cx} f(x)dx = E. \tag{6.4}$$

It might be noted that H is a nonanalytic function of x, but that the Hamilton–Jacobi equation can be solved. Equation (6.4) can be rearranged to yield a solution in quadratures, so that

$$S = \sqrt{2} \int e^{\pm cx} (E - \int^x e^{\pm 2c\bar{x}} f(\bar{x})d\bar{x})^{1/2} dx. \tag{6.5}$$

For this type of separation, $\alpha = E$, so that

$$\beta = \frac{\partial \phi}{\partial \alpha} = \frac{\partial \phi}{\partial E} = \frac{\partial S}{\partial E} - t, \tag{6.6}$$

and

$$\beta + t = \frac{\partial S}{\partial E} = \frac{1}{\sqrt{2}} \int \frac{e^{\pm cx}}{[E - \int^x e^{\pm 2c\bar{x}} f(\bar{x})d\bar{x}]^{1/2}} dx. \tag{6.7}$$

It can be readily shown that (6.7) is in agreement with the solution obtained by direct integration of (6.1).

It is interesting to note that for the equation of motion given by

$$\ddot{x} + c\dot{x}^2 = 0, \tag{6.8}$$

Eq. (6.7) immediately gives the solution

$$t + \beta = \int (e^{cx}/\sqrt{2E})dx, \tag{6.9}$$

or

$$x = (1/c) \ln[\sqrt{2E}\, c(t + \beta)]. \tag{6.10}$$

7. DISCUSSION

The Hamilton–Jacobi equations for a number of simple classical dissipative systems can be solved by the techniques indicated. For single particle systems acted on by linear friction, the Hamilton–Jacobi equation can be separated into space and time components by the substitution

$$\phi(\mathbf{r}, \boldsymbol{\alpha}, t) = e^{\gamma t} Q(\mathbf{r}, \boldsymbol{\alpha}), \tag{7.1}$$

in contrast to the linear separation appropriate to conservative systems

$$\phi(\mathbf{r}, \boldsymbol{\alpha}, t) = S(\mathbf{r}, \boldsymbol{\alpha}) - Et. \tag{7.2}$$

Note that the separation (7.1) is simpler in structure than (7.2) since the α_i are independent in (7.1), while E and the α_i are not independent in (7.2).

The separation (7.1) is actually somewhat more generally applicable than indicated in the previous sections. For a particle moving in a curved metric space with generalized coordinate q^i without dissipation, characterized by the Lagrangian

$$L_0 = \frac{m}{2} g_{ij} \frac{dq^i}{dt} \frac{dq^j}{dt} - V(q^k), \tag{7.3}$$

where g_{ij} is the covariant metric tensor, a linear dissipative force is added to the equation of motion if L_0 is modified to[8]

$$\tilde{L} = e^{\gamma t} L_0. \tag{7.4}$$

Then the corresponding Hamiltonian is

$$\tilde{H} = (e^{-\gamma t}/2m) g^{ij} p_i p_j + V e^{\gamma t}, \tag{7.5}$$

where p_i is the covariant momentum conjugate to q^i. The Hamilton–Jacobi equation corresponding to $\tilde{H}$ is

$$\frac{e^{-\gamma t}}{2m} g^{ij} \frac{\partial \phi}{\partial q^i} \frac{\partial \phi}{\partial q^j} + e^{\gamma t} V(q^k) + \frac{\partial \phi}{\partial t} = 0, \tag{7.6}$$

and the substitution $\phi = e^{\gamma t} Q(q^i, \alpha^i)$ again leads to separation of the t variable.

Surprisingly, the Hamiltonian and the Hamilton–Jacobi equation for the quadratic friction problem of Sec. 6 correspond to those for conservative systems and therefore the additive separation of t *via* (7.2) is sufficient. However, the constant parameter E in this case is *not* the usual energy $T + V$.

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The application of Regge symmetry to the 9-j symbol

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(Received 21 August 1972)

The Regge transposition symmetry is applied to one of the six Wigner coefficients in the defining expression for the Wigner (9-j) symbol; couplings are then performed, and an expression for the (9-j) symbol is obtained which factorizes the sums of the angular momenta in two rows and their differences into different factors.

Recently two new expressions for the Wigner (9-j) symbol have been published: that of Jucys and Ališauskas[1] has the advantage of expressing the most general (9-j) symbol for the first time with only three internal indices of summation, though at considerable expense of explicit symmetry; the expression of Wu,[2] on the other hand, employs six indices of summation and makes all symmetries explicit without the aid of structural units, Wigner or Racah coefficients, in terms of which the (9-j) symbol is usually written.

The present work offers still another expression for the (9-j) symbol; its starting point is given by two questions: (i) What happens to the (9-j) symbol when we apply the Regge transposition symmetry to one of the Wigner coefficients in its defining expression? (ii) Is it possible to obtain an expression for the (9-j) symbol which isolates the dependence of the sums of the angular momenta in two rows and their differences into different factors, i.e., a factorization of the form

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ l_1 & l_2 & l_3 \\ k_1 & k_2 & k_3 \end{Bmatrix} = M(j_i, l_i, k_i) \sum_{\Psi} F(j_i - l_i, k_i, \Psi) G(j_i + l_i, k_i, \Psi), \qquad (1)$$

where M is a monomial factor and Ψ denotes one or more parameters of summation?

When Regge[3] first determined the full symmetry group, of 72 elements, of the $SU(2)$ Wigner coefficient, it was natural to impose the transposition symmetry, i.e., the reflection of the symbol

$$\begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m \end{pmatrix} = \boxed{\begin{matrix} j_2 + j - j_1 & j_1 + j - j_2 & j_1 + j_2 - j \\ j_1 - m_1 & j_2 - m_2 & j - m \\ j_1 + m_1 & j_2 + m_2 & j + m \end{matrix}} \qquad (2)$$

about its diagonal extending from lower left to upper right, on the Wigner coefficients in the defining expression for the Racah coefficient. As a result Regge found a larger symmetry group of 144 elements for this coefficient.[4] It was natural then to impose the transposition symmetry on one of the Wigner coefficients in the defining expression for the (9-j) symbol in the attempt to discover a symmetry group for this symbol of more than 72 elements, for which many have searched without success. The question remains, however, of what properties the (9-j) symbol does indeed show when one of its constituent Wigner coefficients is subjected to the Regge transposition.

In the study of the higher orthogonal groups and their complex extensions we encounter the (9-j) symbol in aspects such that the sums of the angular momenta in two rows and their differences become the "significant" or "useful" parameters rather than the individual angular momenta themselves. E.g., the Wigner coefficient of $SO(4)$ in the $SO(3)$ basis is proportional to the (9-j) symbol, which may be analytically continued in the three sums of the angular momenta in two of its rows to complex values whose real parts are equal to -1 in order to obtain the Wigner coefficient coupling unitary representations of the Lorentz group $SO(3,1)$ in the $SO(3)$ basis. The three differences between the angular momenta in these rows, however, remain fixed; they are not continued, but their absolute magnitudes denote the lowest values of the angular momenta [the invariants of the $SO(3)$ subgroup] occurring in the representations being coupled. Also, (9-j) symbols occur as structural units in the matrix element of a finite transformation in an irreducible representation of $SO(5)$. In the notation of Hecht[5] and the present author,[6,7] we have

$$\begin{aligned} &\langle J_m, \Lambda_m; J', \Lambda'; L' | e^{iL_{45}\theta} | J_m, \Lambda_m; J, \Lambda; L \rangle \\ &= \sum_{\substack{j_1+\lambda_1 = j_1'+\lambda_1' = J_m \\ j_2+\lambda_2 = j_2'+\lambda_2' = \Lambda_m}} \sum_{K_1, K_2} (2K_1+1)(2K_2+1) \\ &\quad \times (-1)^{j_1'+j_2'-J'} \\ &\quad \times C^{\frac{1}{2}(J_m+\Lambda_m-J'-\Lambda') \quad \frac{1}{2}(J_m+\Lambda_m+J'+\Lambda')+1 \quad J_m+\Lambda_m+1}_{\frac{1}{2}(\lambda_1'+\lambda_2'-j_1'-j_2'+J'-\Lambda') \quad \frac{1}{2}(j_1'+j_2'-\lambda_1'-\lambda_2'+J'-\Lambda') \quad J'-\Lambda'} \\ &\quad \times C^{J' \quad \Lambda'}_{j_1'-j_2' \quad \lambda_1'-\lambda_2' \quad J_m-\Lambda_m} \\ &\quad \times [(2J'+1)(2\Lambda'+1)]^{1/2} \begin{Bmatrix} j_1' & \lambda_1' & K_1 \\ j_2' & \lambda_2' & K_2 \\ J' & \Lambda' & L' \end{Bmatrix} d^{K_1}_{j_1'-\lambda_1', j_1-\lambda_1}(\theta) \\ &\quad \times d^{K_2}_{j_2'-\lambda_2', j_2-\lambda_2}(\theta) [(2J+1)(2\Lambda+1)]^{1/2} \\ &\quad \times \begin{Bmatrix} j_1 & \lambda_1 & K_1 \\ j_2 & \lambda_2 & K_2 \\ J & \Lambda & L \end{Bmatrix} (-1)^{j_1+j_2-J} \\ &\quad \times C^{\frac{1}{2}(J_m+\Lambda_m-J-\Lambda) \quad \frac{1}{2}(J_m+\Lambda_m+J+\Lambda)+1 \quad J_m+\Lambda_m+1}_{\frac{1}{2}(\lambda_1+\lambda_2-j_1-j_2+J-\Lambda) \quad \frac{1}{2}(j_1+j_2-\lambda_1-\lambda_2+J-\Lambda) \quad J-\Lambda} \\ &\quad \times C^{J \quad \Lambda}_{j_1-j_2 \quad \lambda_1-\lambda_2 \quad J_m-\Lambda_m} \delta_{L,L'}, \end{aligned} \qquad (3)$$

where (J_m, Λ_m) denotes the maximal weight of the representation of $SO(5)$, (J, Λ) and (J', Λ') the representations of the $SO(4)$ subgroup, and L the representation of the $SO(3)$ subgroup in the chain $SO(5) \supset SO(4) \supset SO(3)$. Here we note that the (9-j) symbol couples two Wigner rotation functions, and that the differences of the first two columns of angular momenta take the place of magnetic quantum numbers of $SO(3)$ Wigner coefficients. The

analogy between the (9-j) symbol and the $SO(3)$ Wigner coefficient has been remarked earlier[7]; in fact, the doubly stretched (9-j) symbol is simply proportional to the $SO(3)$ Wigner coefficient, the three differences of the angular momenta in the stretched columns appearing as the magnetic quantum numbers[8-10]:

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_1+j_3 & j_2+j_4 & j \end{Bmatrix}$$

$$= \left(\frac{(2j_1)!(2j_2)!(2j_3)!(2j_4)!(j_1+j_3+j_2+j_4-j)!}{(2j+1)(2j_1+2j_3+1)!(2j_2+2j_4+1)!}\right.$$

$$\times \left.\frac{(j_1+j_3+j_2+j_4+j+1)!}{(j_1+j_2-j_{12})!(j_1+j_2+j_{12}+1)!}\right)^{1/2}$$

$$\times \left(\frac{1}{(j_3+j_4-j_{34})!(j_3+j_4+j_{34}+1)!}\right)^{1/2}$$

$$\times C^{j_{12}\ j_{34}\ j}_{j_1-j_2\ j_3-j_4\ j_1+j_3-j_2-j_4}, \tag{4}$$

and in the case of a single degeneracy,

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_1+j_3 & j_{24} & j \end{Bmatrix}$$

$$= \left(\frac{(2j_1)!(2j_3)!(j_2+j_{12}-j_1)!(j_2+j_4-j_{24})!}{(2j+1)(2j_1+2j_3+1)!(j_{12}-j_2+j_1)!}\right.$$

$$\times \left.\frac{(j_4+j_{34}-j_3)!(j_1+j_3+j_{24}-j)!}{(j_1+j_2-j_{12})!(j_1+j_2+j_{12}+1)!}\right)^{1/2}$$

$$\times \left(\frac{(j_1+j_3+j_{24}+j+1)!}{(j_2-j_4+j_{24})!(-j_2+j_4+j_{24})!(j_2+j_4+j_{24}+1)!}\right.$$

$$\times \left.\frac{1}{(j_3-j_4+j_{34})!(j_3+j_4-j_{34})!(j_3+j_4+j_{34}+1)!}\right)^{1/2}$$

$$\times \sum_y (-1)^y \frac{(2j_4-y)!(j_2-j_4+j_{24}+y)!}{y!(j_2+j_4-j_{24}-y)!}$$

$$\times \left(\frac{(j_{12}+j_4+j_1-j_{24}-y)!(j_{34}-j_4+j_3+y)!}{(j_{12}-j_4-j_1+j_{24}+y)!(j_{34}+j_4-j_3-y)!}\right)^{1/2}$$

$$\times C^{j_{12}\ j_{34}\ j}_{j_4+j_1-j_{24}-y\ j_3-j_4+y\ j_1+j_3-j_{24}}. \tag{5}$$

And, of course, the $SO(3)$ Wigner coefficient and the (9-j) symbol have isomorphic symmetry groups of 72 elements.

In answer to both of the questions which we have posed above we assert the identity

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = (-1)^{j+j_{13}+j_{24}} \left(\frac{(j_1+j_3-j_{13})!(j_1+j_3+j_{13}+1)!(j_2+j_4-j_{24})!(j_2+j_4+j_{24}+1)!}{(2j+1)(2j_{13}+1)(2j_{24}+1)}\right)^{1/2}$$

$$\times [(j_{12}+j_{34}-j)!(j_{12}+j_{34}+j+1)!]^{1/2}\,\Delta(j_1j_2j_{12})\Delta(j_3j_4j_{34}) \sum_{\Psi_1\Psi_2\Psi_3} (2\Psi_1+1)(2\Psi_2+1)(2\Psi_3+1)$$

$$\times \frac{1}{[\frac{1}{2}(j_2+j_4+j_{12}+j_{34}-j_1-j_3)-\Psi_1]![\frac{1}{2}(j_2+j_4+j_{12}+j_{34}-j_1-j_3)+\Psi_1+1]!}$$

$$\times \frac{1}{[\frac{1}{2}(j_{12}+j_{34}+j_1+j_3-j_2-j_4)-\Psi_2]![\frac{1}{2}(j_{12}+j_{34}+j_1+j_3-j_2-j_4)+\Psi_2+1]!}$$

$$\times \frac{1}{[\frac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34})-\Psi_3]![\frac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34})+\Psi_3+1]!}$$

$$\times \begin{Bmatrix} j_{13} & j_{24} & j \\ \Psi_1 & \Psi_2 & \Psi_3 \end{Bmatrix} C^{\Psi_3\ \Psi_2\ j_{13}}_{\frac{1}{2}(j_1-j_3+j_2-j_4-j_{12}+j_{34})\ \frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34})\ j_1-j_3} C^{\Psi_1\ \Psi_3\ \Psi_{24}}_{\frac{1}{2}(-j_1+j_3+j_2-j_4+j_{12}-j_{34})\ \frac{1}{2}(j_1-j_3+j_2-j_4-j_{12}+j_{34})\ j_2-j_4}$$

$$\times C^{\Psi_2\ \Psi_1\ j}_{\frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34})\ \frac{1}{2}(-j_1+j_3+j_2-j_4+j_{12}-j_{34})\ j_{12}-j_{34}}$$

$$= (-1)^{j+j_{13}+j_{24}} \left(\frac{(2j_1+1)!(2j_3+1)!(2j_2+1)!(2j_4+1)!}{(j_1+j_2-j_{12})!(j_1-j_2+j_{12})!(-j_1+j_2+j_{12})!(j_1+j_2+j_{12}+1)!(j_3+j_4-j_{34})!}\right)^{1/2}$$

$$\times \left(\frac{(2j_{12}+1)!(2j_{34}+1)!}{(j_3-j_4+j_{34})!(-j_3+j_4+j_{34})!(j_3+j_4+j_{34}+1)!}\right)^{1/2} \sum_{\Psi_1\Psi_2\Psi_3} (2\Psi_1+1)(2\Psi_2+1)(2\Psi_3+1)$$

$$\times \begin{Bmatrix} j_{13} & j_{24} & j \\ \Psi_1 & \Psi_2 & \Psi_3 \end{Bmatrix} \begin{Bmatrix} \frac{1}{2}(j_1+j_2-j_{12}) & \frac{1}{2}(j_3+j_4-j_{34}) & \Psi_3 \\ \frac{1}{2}(j_1-j_2+j_{12}) & \frac{1}{2}(j_3-j_4+j_{34}) & \Psi_2 \\ j_1 & j_3 & j_{13} \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(-j_1+j_2+j_{12}) & \frac{1}{2}(-j_3+j_4+j_{34}) & \Psi_1 \\ \frac{1}{2}(j_1+j_2-j_{12}) & \frac{1}{2}(j_3+j_4-j_{34}) & \Psi_3 \\ j_2 & j_4 & j_{24} \end{Bmatrix} \begin{Bmatrix} \frac{1}{2}(j_1-j_2+j_{12}) & \frac{1}{2}(j_3-j_4+j_{34}) & \Psi_2 \\ \frac{1}{2}(-j_1+j_2+j_{12}) & \frac{1}{2}(-j_3+j_4+j_{34}) & \Psi_1 \\ j_{12} & j_{34} & j \end{Bmatrix}. \tag{6}$$

We note that the first of these two expressions for the (9-j) symbol isolates the dependence on the three differences between angular momenta of the first two columns into the monomial factor and the magnetic quantum numbers of the three $SU(2)$ Wigner coefficients. We may prove this identity very easily: First we expand any two of the doubly stretched (9-j) symbols on the right of (6) in (6-j) symbols:

$$\begin{Bmatrix} \frac{1}{2}(j_2-j_1+j_{12}) & \frac{1}{2}(j_4-j_3+j_{34}) & \Psi_1 \\ \frac{1}{2}(j_1+j_2-j_{12}) & \frac{1}{2}(j_3+j_4-j_{34}) & \Psi_3 \\ j_2 & j_4 & j_{24} \end{Bmatrix}$$

$$= \sum_q (2q+1)(-1)^{2q} \begin{Bmatrix} \frac{1}{2}(j_3+j_4-j_{34}) & \frac{1}{2}(j_1+j_2-j_{12}) & \Psi_3 \\ q & \frac{1}{2}(j_4-j_3+j_{34}) & j_4 \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_4-j_3+j_{34}) & \frac{1}{2}(j_2-j_1+j_{12}) & \Psi_1 \\ j_{24} & \Psi_3 & q \end{Bmatrix}$$

$$\times \begin{Bmatrix} j_4 & j_2 & j_{24} \\ \frac{1}{2}(j_2-j_1+j_{12}) & q & \frac{1}{2}(j_1+j_2-j_{12}) \end{Bmatrix},$$

$$\begin{Bmatrix} \frac{1}{2}(j_1+j_2-j_{12}) & \frac{1}{2}(j_3+j_4-j_{34}) & \Psi_3 \\ \frac{1}{2}(j_1-j_2+j_{12}) & \frac{1}{2}(j_3-j_4+j_{34}) & \Psi_2 \\ j_1 & j_3 & j_{13} \end{Bmatrix}$$

$$= (-1)^{\Psi_3+\Psi_2-j_{13}} \sum_{q'} (2q'+1)(-1)^{2q'}$$

$$\times \begin{Bmatrix} j_3 & j_1 & j_{13} \\ \frac{1}{2}(j_1-j_2+j_{12}) & q' & \frac{1}{2}(j_1+j_2-j_{12}) \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_3+j_4-j_{34}) & \frac{1}{2}(j_1+j_2-j_{12}) & \Psi_3 \\ \Psi_2 & j_{13} & q' \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_3-j_4+j_{34}) & \frac{1}{2}(j_1-j_2+j_{12}) & \Psi_2 \\ j_{13} & \Psi_3 & q' \end{Bmatrix}. \tag{7}$$

We start from the expression

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = \left(\frac{(j_{13}+j_{24}+j+1)!(j_{13}-j_{24}+j)!(j_1+j_3-j_{13})!(j_{12}+j_{34}-j)!(j_1+j_2-j_{12})!}{(2j_{24}+1)(j_1+j_3+j_{13}+1)!(j_1-j_3+j_{13})!(-j_1+j_3+j_{13})!(j_{12}+j_{34}+j+1)!} \right)^{1/2}$$

$$\times \left(\frac{(j_1-j_2+j_{12})!(-j_1+j_2+j_{12})!(j_3+j_4-j_{34})!(j_3-j_4+j_{34})!(-j_3+j_4+j_{34})!}{(j_{12}-j_{34}+j)!(-j_{12}+j_{34}+j)!(j_1+j_2+j_{12}+1)!(j_3+j_4+j_{34}+1)!} \right)^{1/2}$$

$$\times \sum_{\substack{m_1 m_2 \\ z_1 z_2}} (-1)^{-j_{12}-j_3+j_{13}+m_2+z_1+z_2}$$

$$\times \frac{[(j_2+m_2)!(j_2-m_2)!(j_4+j-j_{13}-m_2)!(j_4-j+j_{13}+m_2)!]^{1/2}(j_1+m_1)!}{z_1!(j_1-m_1-z_1)!(j_2-j_1+m_1+m_2+z_1)!(j_2-j_{12}+m_1+z_1)!(j_{12}-m_1-m_2-z_1)!}$$

$$\times \frac{(j_3+j_{13}-m_1)!(j_{12}+m_1+m_2)!(j_{34}+j-m_1-m_2)!}{(j_{12}+j_1-j_2-z_1)!z_2!(j_3-j_{13}+m_1-z_2)!(j_4-j_3+j-m_1-m_2+z_2)!(j_4-j_{34}+j_{13}-m_1+z_2)!}$$

We now sum over the angular momenta Ψ_1 and Ψ_2 applying the identity[11]

$$\sum_{j_{13}j'_{13}} (2j_{13}+1)(2j'_{13}+1)(-1)^{j'_{13}+j_2+j_3-j'_{12}-k_1+2j'_3}$$

$$\times \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_4 & j_3 & j_{13} \end{Bmatrix} \begin{Bmatrix} j'_1 & j'_2 & j'_{12} \\ j_4 & j'_3 & j'_{13} \end{Bmatrix} \begin{Bmatrix} j'_{13} & j'_2 & j_4 \\ j_2 & j_{13} & k_2 \end{Bmatrix} \begin{Bmatrix} j'_1 & j'_3 & j'_{13} \\ j_1 & j_3 & j_{13} \\ k_1 & k_3 & k_2 \end{Bmatrix}$$

$$= \begin{Bmatrix} j'_{12} & j'_3 & j_4 \\ j_3 & j_{12} & k_3 \end{Bmatrix} \begin{Bmatrix} j'_1 & j'_2 & j'_{12} \\ j_1 & j_2 & j_{12} \\ k_1 & k_2 & k_3 \end{Bmatrix}, \tag{8}$$

then perform the sum over Ψ_3 by means of the Biedenharn–Elliott identity, then sum over q and q' by means of the identity (8). The result is the original (9-j) symbol multiplied by degenerate (6-j) symbols which are the multiplicative inverse of the coefficient factor before the summation sign on the right-hand side of (6). Hence the identity (6) is established.

It is worthwhile, however, to trace the derivation of (6), since the process may be paradigmatic for the derivation of similar identities for the coefficients recoupling four irreducible representations of groups other than $SU(2)$. The identity (6) allows us to factorize matrix elements of tensor operators in the orbital group $Sp(4)*Sp(4)$ into a sum over products of (noncanonical) $Sp(4)$ coupling coefficients.[12] Similarly, matrix elements of tensor operators in $U(n)*U(n)$ consist of two "(9-j) symbols" in $U(n-1)$ coupled with three matrix elements of totally symmetric operators in $U(n)$. Since the identity (6), applied to the (9-j) symbols in the $SO(4) \times SO(4)$ subgroup of the $Sp(4)*Sp(4)$ matrix element, allows us to perform a factorization, we may speculate that analogous identities on the (9-j) symbols of $U(n-1)$ will allow us to factorize $U(n)*U(n)$ matrix elements in similar manner. Hence we shall investigate the derivation of (6) in detail.

$$\times \frac{1}{(j_{34}-j+m_1+m_2-z_2)!}$$

$$\times \frac{1}{(j_{34}+j_3-j_4-z_2)!}\, C^{\frac{1}{2}(j_2+j_4+j-j_{13})\quad \frac{1}{2}(j_2+j_4-j+j_{13})\quad j_{24}}_{\frac{1}{2}(j_2-j_4-j+j_{13})+m_2\ \frac{1}{2}(j_2-j_4+j-j_{13})-m_2\ j_2-j_4}, \tag{9}$$

where we have applied the Regge transposition symmetry

$$C^{j_2\ j_4\ j_{24}}_{m_2\ j-j_{13}-m_2\ j-j_{13}} = C^{\frac{1}{2}(j_2+j_4+j-j_{13})\quad \frac{1}{2}(j_2+j_4-j+j_{13})\quad j_{24}}_{\frac{1}{2}(j_2-j_4-j+j_{13})+m_2\ \frac{1}{2}(j_2-j_4+j-j_{13})-m_2\ j_2-j_4}. \tag{10}$$

We now extract from the other factors under the summation sign the degenerate Wigner coefficients

$$C^{\frac{1}{2}(j_2+j_4+j-j_{13})\quad \frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2)\quad \frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2)}_{\frac{1}{2}(j_2-j_4-j+j_{13})+m_2\ \frac{1}{2}(-j_1+j_3-j_{13}+z_1-z_2)+m_1\ \frac{1}{2}(j_2-j_4-j_1+j_3-j+z_1-z_2)+m_1+m_2}$$

$$\times C^{\frac{1}{2}(j_2+j_4-j+j_{13})\quad \frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2)\quad \frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2)}_{\frac{1}{2}(j_2-j_4+j-j_{13})-m_2\ \frac{1}{2}(-j_2+j_4+j_{12}-j_{34}+j_{13}-z_1+z_2)-m_1\ \frac{1}{2}(j_{12}-j_{34}+j-z_1+z_2)-m_1-m_2}, \tag{11}$$

and we write the product of the three coefficients (10) and (11) in the form

$$\sum_{\Psi_1\Psi_3} [(j_2+j_4-j_1-j_3+j+z_1+z_2+1)(j_{12}+j_{34}-j-z_1-z_2+1)(2j_{24}+1)(2\Psi_3+1)]^{1/2}$$

$$\times C^{\frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2)\quad \frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2)\quad \Psi_3}_{\frac{1}{2}(-j_1+j_3-j_{13}+z_1-z_2)+m_1\ \frac{1}{2}(-j_2+j_4+j_{12}-j_{34}+j_{13}-z_1+z_2)-m_1\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})}$$

$$\times C^{\frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2)\quad \frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2)\quad \Psi_1}_{\frac{1}{2}(j_2-j_4-j_1+j_3-j+z_1-z_2)+m_1+m_2\ \frac{1}{2}(j_{12}-j_{34}+j-z_1+z_2)-m_1-m_2\ \frac{1}{2}(j_2-j_4-j_1+j_3+j_{12}-j_{34})}$$

$$\times C^{j_{24}\quad \Psi_3\quad \Psi_1}_{j_2-j_4\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})\ \frac{1}{2}(-j_1+j_3+j_2-j_4+j_{12}-j_{34})}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_2+j_4+j-j_{13}) & \frac{1}{2}(j_2+j_4-j+j_{13}) & j_{24} \\ \frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2) & \frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2) & \Psi_3 \\ \frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2) & \frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2) & \Psi_1 \end{Bmatrix}. \tag{12}$$

From the remaining factors we form the degenerate Wigner coefficients

$$C^{\frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2)\quad \frac{1}{2}(j_1+j_3+j_{13})\quad j_{13}+\frac{1}{2}(z_1+z_2)}_{\frac{1}{2}(-j_1+j_3-j_{13}+z_1-z_2)+m_1\ \frac{1}{2}(-j_1+j_3+j_{13})-m_1\ -j_1+j_3+\frac{1}{2}(z_1-z_2)}\, C^{\frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2)\quad \frac{1}{2}(j_1+j_3+j_{13})\quad \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)}_{\frac{1}{2}(-j_2+j_4+j_{12}-j_{34}+j_{13}-z_1+z_2)-m_1\ \frac{1}{2}(j_1-j_3-j_{13})+m_1\ \frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34}-z_1+z_2)}$$

$$\times C^{\frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2)\quad \frac{1}{2}(j_{12}+j_{34}+j)\quad \frac{1}{2}(j_1+j_3+j_{12}+j_{34}-j_2-j_4-z_1-z_2)}_{\frac{1}{2}(j_2-j_4-j_1+j_3-j+z_1-z_2)+m_1+m_2\ \frac{1}{2}(-j_{12}+j_{34}+j)-m_1-m_2\ \frac{1}{2}(-j_{12}+j_{34}-j_1+j_3+j_2-j_4+z_1-z_2)}$$

$$\times C^{\frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2)\quad \frac{1}{2}(j_{12}+j_{34}+j)\quad j+\frac{1}{2}(z_1+z_2)}_{\frac{1}{2}(j_{12}-j_{34}+j-z_1+z_2)-m_1-m_2\ \frac{1}{2}(j_{12}-j_{34}-j)+m_1+m_2\ j_{12}-j_{34}-\frac{1}{2}(z_1-z_2)}, \tag{13}$$

and sum over m_1 and m_2 to obtain

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} = A \sum_{\substack{z_1 z_2 \\ \Psi_1\Psi_3}} (-1)^{-j_{12}+j_4-j_3+j+2\Psi_1+2\Psi_3+z_1+z_2} \frac{(j_1+j_3+j_{13}+1)!\,(j_{12}+j_{34}+j+1)!}{(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)!}$$

$$\times \frac{[(2j_{24}+1)(2\Psi_3+1)]^{1/2}}{(j_1+j_3-j_{13}-z_1-z_2)!\,(j_2+j_4-j_1-j_3+j+z_1+z_2)!}$$

$$\times \frac{1}{(j_{12}+j_{34}-j-z_1-z_2)!\,(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2)!}$$

$$\times \left(\frac{(j_2+j_4+j-j_{13}+1)!\,(j_2+j_4-j+j_{13}+1)!}{(2j_{13}+z_1+z_2)!\,(2j+z_1+z_2)!}\right)^{1/2} C^{j_{24}\quad \Psi_3\quad \Psi_1}_{j_2-j_4\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})\ \frac{1}{2}(-j_1+j_3+j_2-j_4+j_{12}-j_{34})}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_2+j_4+j-j_{13}) & \frac{1}{2}(j_2+j_4-j+j_{13}) & j_{24} \\ \frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2) & \frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2) & \Psi_3 \\ \frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2) & \frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2) & \Psi_1 \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_2+j_4-j_{12}-j_{34}+j_{13}+z_1+z_2) & \frac{1}{2}(j_1+j_3+j_{13}) & \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2) \\ j_{13}+\frac{1}{2}(z_1+z_2) & \Psi_3 & \frac{1}{2}(j_1+j_3-j_{13}-z_1-z_2) \end{Bmatrix}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_{12}+j_{34}-j-z_1-z_2) & \frac{1}{2}(j_{12}+j_{34}+j) & j+\frac{1}{2}(z_1+z_2) \\ \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2) & \Psi_1 & \frac{1}{2}(j_2+j_4-j_1-j_3+j+z_1+z_2) \end{Bmatrix}$$

$$\times \left\{ \frac{1}{z_1!\,z_2!} [(j_1+j_{13}-j_3+z_2)!\,(j_{13}+j_3-j_1+z_1)!\,(j_{12}-j_{34}+j+z_2)!\,(j+j_{34}-j_{12}+z_1)!]^{1/2} \right.$$

$$\times C^{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)\ j_{13}+\frac{1}{2}(z_1+z_2)\ \Psi_3}_{\frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34}-z_1+z_2)\ j_3-j_1+\frac{1}{2}(z_1-z_2)\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})}$$

$$\left. \times C^{j+\frac{1}{2}(z_1+z_2)\ \ \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)\ \ \Psi_1}_{j_{12}-j_{34}-\frac{1}{2}(z_1-z_2)\ \frac{1}{2}(-j_1+j_3+j_2-j_4-j_{12}+j_{34}+z_1-z_2)\ \frac{1}{2}(-j_1+j_3+j_2-j_4+j_{12}-j_{34})} \right\}, \tag{14}$$

where A denotes the constant before the summation sign in (9). The factor in curly brackets at the end of the right-hand side of (14) can be written as

$$\sum_{z_1-z_2} C^{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)\ j_{13}+\frac{1}{2}(z_1+z_2)\ \Psi_3}_{\frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34}-z_1+z_2)\ j_3-j_1+\frac{1}{2}(z_1-z_2)\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})}$$

$$\times C^{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2)\ j+\frac{1}{2}(z_1+z_2)\ \Psi_1}_{\frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34}-z_1+z_2)\ -j_{12}+j_{34}+\frac{1}{2}(z_1-z_2)\ \frac{1}{2}(j_1-j_3-j_2+j_4-j_{12}+j_{34})}$$

$$\times C^{j_{13}+\frac{1}{2}(z_1+z_2)\ \ \frac{1}{2}(z_1+z_2)\ j_{13}}_{-j_1+j_3+\frac{1}{2}(z_1-z_2)\ -\frac{1}{2}(z_1-z_2)\ -j_1+j_3} C^{j+\frac{1}{2}(z_1+z_2)\ \ \frac{1}{2}(z_1+z_2)\ j}_{-j_{12}+j_{34}+\frac{1}{2}(z_1-z_2)\ -\frac{1}{2}(z_1-z_2)\ -j_{12}+j_{34}}$$

$$\times \frac{1}{(z_1+z_2)!} \left(\frac{(j_{13}+j_1-j_3)!\,(j_{13}-j_1+j_3)!\,(j-j_{12}+j_{34})!}{(j+j_{12}-j_{34})!\,(2j_{13}+z_1+z_2+1)!\,(2j+z_1+z_2+1)!} \right)^{1/2}$$

$$= \frac{1}{(z_1+z_2)!} \left(\frac{(j_{13}+j_1-j_3)!\,(j_{13}-j_1+j_3)!\,(j+j_{12}-j_{34})!\,(j-j_{12}+j_{34})!\,(2j_{13}+z_1+z_2+1)!\,(2j+z_1+z_2+1)!}{(2j+1)!\,(2j_{13}+1)!} \right)^{1/2}$$

$$\times \sum_q [(2\Psi_3+1)(2\Psi_1+1)(2j+1)(2j_{13}+1)]^{1/2} C^{\Psi_3\ \ \ j\ \ \ q}_{\frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})\ -j_{12}+j_{34}\ \frac{1}{2}(-j_1+j_3-j_2+j_4-j_{12}+j_{34})}$$

$$\times C^{\Psi_1\ \ \ j_{13}\ \ q}_{\frac{1}{2}(j_1-j_3-j_2+j_4-j_{12}+j_{34})\ -j_1+j_3\ \frac{1}{2}(-j_1+j_3-j_2+j_4-j_{12}+j_{34})}$$

$$\times \begin{Bmatrix} \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2) & j_{13}+\frac{1}{2}(z_1+z_2) & \Psi_3 \\ j+\frac{1}{2}(z_1+z_2) & \frac{1}{2}(z_1+z_2) & j \\ \Psi_1 & j_{13} & q \end{Bmatrix}$$

$$= \frac{1}{(z_1+z_2)!} \left(\frac{(j_{13}+j_1-j_3)!\,(j_{13}-j_1+j_3)!\,(j+j_{12}-j_{34})!\,(j-j_{12}+j_{34})!\,(2j_{13}+z_1+z_2+1)!\,(2j+z_1+z_2+1)!}{(2j)!\,(2j_{13})!} \right)^{1/2}$$

$$\times \sum_{\Psi_2} [(2\Psi_1+1)(2\Psi_3+1)]^{1/2} (-1)^{j-j_{13}+j_3-j_1+j_{12}-j_{34}+2\Psi_1+2\Psi_3}$$

$$\times \begin{Bmatrix} j+\frac{1}{2}(z_1+z_2) & \frac{1}{2}(z_1+z_2) & j \\ \Psi_2 & \Psi_1 & \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2) \end{Bmatrix}$$

$$\times \begin{Bmatrix} \tfrac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}-z_1-z_2) & j_{13} & \tfrac{1}{2}(z_1+z_2) \\ j_{13} & \Psi_2 & \tfrac{1}{2}(z_1+z_2) \end{Bmatrix} \Psi_3$$

$$\times C^{\Psi_1 \quad j \quad \Psi_2}_{\frac{1}{2}(-j_{12}+j_{34}+j_1-j_3-j_2+j_4)\; j_{12}-j_{34}\; \frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34})} C^{\Psi_3 \quad j_{13} \quad \Psi_2}_{\frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})\; j_1-j_3\; \frac{1}{2}(j_1-j_3-j_2+j_4+j_{12}-j_{34})}. \tag{15}$$

Substituting (15) for the corresponding factor in (14), we note that the four (6-j) symbols are all monomials, and the (9-j) symbol indicated in (14) is doubly stretched so that we may apply the identity (4) to it. We have summed over $z_1 - z_2$ in (15). It remains only to perform the summation over $z_1 + z_2$; this sum now has the form

$$\sum_{z_1+z_2} (-1)^{z_1+z_2}$$

$$\times \left(\frac{[\Psi_1 + j - \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) + z_1 + z_2]! [\Psi_3 + j_{13} - \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) + z_1 + z_2]!}{[\Psi_1 - j + \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) - z_1 - z_2]! [\Psi_3 - j_{13} + \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) - z_1 - z_2]!} \right)^{1/2}$$

$$\times \frac{[\Psi_2 + \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) - z_1 - z_2]!}{[\Psi_2 - \frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) + z_1 + z_2]!} C^{\Psi_3 \quad \Psi_1 \quad j_{24}}_{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34})-j_{13}-z_1-z_2\; -\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34})+j+z_1+z_2\; j-j_{13}} \tag{16}$$

which is simply proportional to the (6-j) symbol

$$\begin{Bmatrix} j_{13} & j_{24} & j \\ \Psi_1 & \Psi_2 & \Psi_3 \end{Bmatrix}. \tag{17}$$

Thus, we have obtained the identity (6).

We note that when the (9-j) symbol has a single degeneracy, as in (5) above, the identity (6) is greatly simplified, i.e., it becomes a sum over a single angular momentum rather than one over three. From (5) above we have

$$\sum_y (-1)^y \frac{(2j_4-y)!(j_2-j_4+j_{24}+y)!}{y!(j_2+j_4-j_{24}-y)!} \left(\frac{(j_{12}+j_4+j_1-j_{24}-y)!(j_{34}-j_4+j_3+y)!}{(j_{12}-j_4-j_1+j_{24}+y)!(j_{34}+j_4-j_3-y)!} \right)^{1/2} C^{j_{12} \quad j_{34} \quad j}_{j_4+j_1-j_{24}-y\; j_3-j_4+y\; j_1+j_3-j_{24}}$$

$$= (-1)^{j_{24}+j_{34}-j_3-j_2}$$

$$\times \left(\frac{(j_{24}+j_4-j_2)!(j_{24}-j_4+j_2)!(j_3+j_4-j_{34})!(j_1+j_2-j_{12})!(j_1-j_2+j_{12})!(j_3-j_4+j_{34})!(2j+1)}{(2j_{24})!(j_1+j_3+j_2+j_4-j_{12}-j_{34})!(j_1+j_3-j_2-j_4+j_{12}+j_{34})!(-j_1-j_3+j_{12}+j_{34}+j_{24})!} \right)^{1/2}$$

$$\times [(j_1+j_3+j_{12}+j_{34}-j_{24}+1)!]^{1/2} \frac{(j_2+j_4+j_{24}+1)!}{(j_2+j_4-j_{24})!} \sum_q C^{j \quad j_{24} \quad q}_{j_{12}-j_{34}\; j_4-j_2\; j_{12}-j_{34}+j_4-j_2}$$

$$\times C^{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34})\; \frac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34}) \quad q}_{\frac{1}{2}(j_{12}-j_{34}+j_1-j_3-j_2+j_4)\; \frac{1}{2}(j_{12}-j_{34}-j_1+j_3-j_2+j_4)\; j_{12}-j_{34}+j_4-j_2}$$

$$\times \begin{Bmatrix} \tfrac{1}{2}(j_1+j_3+j_{12}+j_{34}-j_{24}) & \tfrac{1}{2}(j_{12}+j_{34}-j_1-j_3+j_{24}) & j \\ \tfrac{1}{2}(j_2+j_4-j_{24}) & \tfrac{1}{2}(j_2+j_4+j_{24}) & j_{24} \\ \tfrac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) & \tfrac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34}) & q \end{Bmatrix}$$

$$= (-1)^{j_1+j_3+j_{24}+j_{34}-j_{12}}$$

$$\times \left(\frac{(-j_2+j_4+j_{24})!(j_2-j_4+j_{24})!(j_3+j_4-j_{34})!(j_3-j_4+j_{34})!(j_1-j_2+j_{12})!(j_1+j_2-j_{12})!}{(2j_{24})!(j_1+j_3+j_2+j_4-j_{12}-j_{34}+1)!(j_1+j_3-j_2-j_4+j_{12}+j_{34})!(-j_1-j_3+j_{12}+j_{34}+j_{24})!} \right)^{1/2}$$

$$\times [(2j+1)(j_1+j_3+j_{12}+j_{34}-j_{24}+1)!]^{1/2} \frac{(j_2+j_4+j_{24}+1)!}{(j_2+j_4-j_{24})!} \sum_\Psi \sqrt{2\Psi+1}\,(-1)^{2\Psi}$$

$$\times \begin{Bmatrix} \tfrac{1}{2}(j_1+j_3+j_{12}+j_{34}-j_{24}) & \tfrac{1}{2}(-j_1-j_3+j_{12}+j_{34}+j_{24}) & j \\ \tfrac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34}) & \Psi & \tfrac{1}{2}(j_2+j_4+j_{24}) \end{Bmatrix}$$

$$\times \begin{Bmatrix} \tfrac{1}{2}(j_2+j_4-j_{24}) & \tfrac{1}{2}(j_2+j_4+j_{24}) & j_{24} \\ \Psi & \tfrac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34}) & \tfrac{1}{2}(j_1+j_3+j_{12}+j_{34}-j_{24}) \end{Bmatrix}$$

$$\times C^{\frac{1}{2}(j_1+j_3-j_2-j_4+j_{12}+j_{34})\quad j_{24}\quad \Psi}_{\frac{1}{2}(-j_1+j_3+j_2-j_4-j_{12}+j_{34})\ j_4-j_2\ \frac{1}{2}(-j_1+j_3-j_2+j_4-j_{12}+j_{34})} C^{\Psi\quad j\quad \frac{1}{2}(j_1+j_3+j_2+j_4-j_{12}-j_{34})}_{\frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})\ j_{12}-j_{34}\ \frac{1}{2}(-j_1+j_3-j_2+j_4+j_{12}-j_{34})}. \tag{18}$$

Hence the introduction of this single degeneracy into (6) causes the suppression of four of the seven internal indices of summation.

The analytic continuation of the (9-j) symbol to the Wigner coefficient of the Lorentz group $SO(3,1)$ in its $SO(3)$ basis is accomplished by the substitutions

$$\begin{aligned} j_1 + j_3 &\to -1 + i\rho, \\ j_2 + j_4 &\to -1 + i\rho', \\ j_{12} + j_{34} &\to -1 + i\rho'', \end{aligned} \tag{19}$$

where ρ, ρ', ρ'' are all finite real numbers. We observe that in the parametrization (6) the continuation is especially easy. The sums over Ψ_1, Ψ_2, Ψ_3 become nonterminating but convergent, and no continuation is necessary for any of the parameters in the indicated Wigner or Racah coefficients. It is tempting, then, to speculate that (6) may provide a valid parametrization for the analytic continuation to the Wigner coefficient of $SO(3,1)$; but at present this remains a conjecture.

ACKNOWLEDGMENT

The author would like to thank Professor Wesley E. Brittin for his kind hospitality at the University of Colorado.

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The solution of the moment equations associated with a partial differential equation with polynomial coefficients*

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(Received 30 September 1971; final revised manuscript received 15 September 1972)

In this paper it is shown that the moment equations associated with a partial differential equation with polynomial coefficients possess formal power series solutions which are easily computed. An application is made to an equation which arises in the quantum theory of the laser. A simple example is given which illustrates the fact that although the original differential equation may not be solvable by power series methods, the related moment equations are always solvable.

1. INTRODUCTION

In 1967, Gordon derived an equation which describes the time evolution of a fully quantal model laser in terms of a phase space distribution function $P(x, t)$ of six real variables characterizing the atomic and field systems of the laser.[1] The equation is of the form of the Fokker–Plank equation familiar from the classical theory of stochastic processes, i.e.,

$$\frac{\partial P}{\partial t} = LP, \tag{1.1}$$

$$L = -\sum \frac{\partial}{\partial x_i} A_i(x) + \frac{1}{2}\sum \frac{\partial}{\partial x_i \partial x_j} D_{ij}(x), \quad x = (x_1, \ldots, x_6),$$

but has a nonpositive definite diffusion matrix $D_{ij}(x)$. This makes Eq. (1.1) impossible to solve using standard techniques.[2] The terminology pseudo-Fokker–Plank (PFP) has been introduced to characterize equations of this type.[3] (For a discussion of the "physics" underlying the occurrence of PFP equations, see Ref. 4). Although the PFP equation characterizing a quantal model of a lossless parametric amplifier has been solved,[3,5] no solutions of Gordon's equation are presently known. However, one may derive useful information, e.g., the coherence properties of the laser field, from the moment equations associated with (1.1), and it is therefore of interest to examine the question of existence of solutions of these moment equations.

In the cases we wish to consider, the drift and diffusion matrices, $A_i(x)$ and $D_{ij}(x)$, are polynomials, and the associated moment equations form an infinite system of first order ordinary differential equations with constant coefficients. We show that all such systems have a unique formal power series solution which can be explicitly computed. The possible convergence of the formal power series is a difficult question[6] which we do not attempt to answer in this paper. With special assumptions about the form operator L in (1.1), the related moment equations have been studied previously.[7,8] However, in many interesting cases the conditions needed to apply the results of these investigations are not satisfied. A particular case in point is Gordon's equation,[1] an equation to which our theory does apply.

In Sec. 2 we consider an equation of the form (1.1) where L is an arbitrary differential operator in one variable with polynomial coefficients. We show that the related moment equations are of strip type. We then proceed to show that even more general infinite systems of ordinary differential equations also have formal power series solutions. In Sec. 3 we generalize the results of Sec. 2 to the case of n variables, and then show how to solve the moment equations associated to Gordon's equation. In Sec. 4 we give an example of a differential equation which does not possess an analytic solution but whose moment equations are solvable. This indicates that it is possible to solve the moment equations when the original differential equations are not solvable.

2. THE MOMENT EQUATIONS

In this section we are going to show that the moment equations associated with a differential equation, with polynomial coefficients, are of a special type called strip type. We then show how to solve even more general infinite systems of ordinary differential equations of semilower diagonal type. Since the n variable case is a straightforward generalization of the one variable case, we first discuss the latter. Let

$$L(x, \xi) = \sum_{i=0, j=0}^{\alpha, \beta} a_{ij} x^i \xi^j \tag{2.1}$$

be a polynomial in two variables, and then let

$$L\left(x, \frac{d}{dx}\right) = \sum_{ij} a_{ij} x^i \left(\frac{d}{dx}\right)^j. \tag{2.2}$$

If we assume that $v(x)$ is sufficiently nice (say integrable with bounded support), then we define the nth moment v_n of v by

$$v_n = \langle v, x^n \rangle = \int_{-\infty}^{\infty} v(x) x^n dx. \tag{2.3}$$

We also note that

$$\left\langle x^i \left(\frac{d}{dx}\right)^j v(x), x^n \right\rangle = \left\langle v(x), \frac{(-1)^j (n+i)!}{(n+1-j)!} x^{n+i-j} \right\rangle, \tag{2.4}$$

where we have integrated by parts. Now, if $P(x, t)$ satisfies

$$\frac{\partial P}{\partial t} = L\left(x, \frac{d}{dx}\right) P, \qquad P(x, 0) = f(x) \tag{2.5}$$

and

$$P_n(t) = \langle P(x, t), x^n \rangle, \qquad f_n = \langle f(x), x^n \rangle, \tag{2.6}$$

then $P_n(t)$ should satisfy the infinite system of ordinary differential equations,

$$P_n'(t) = \frac{dP_n(t)}{dt} = \sum a_{ij}(-1)^j \frac{(n+i)!}{(n+i-j)!} P_{(n+i-j)}(t), \qquad P_n(0) = f_n \tag{2.7}$$

where $0 \le i \le \alpha$, $0 \le j \le \min(n+i, \beta)$.

Remark: This is a purely formal derivation. It is entirely possible that the original equation may have a solution which has no finite moments. It is also possible that the moment equations possess a solution when the original equation does not. We now try to solve the moment equations, forgetting from whence they came.

We can write our Eq. (2.7) as

$$P_m'(t) = \sum A_{mn} P_n(t), \qquad P_m(0) = f_m, \tag{2.8}$$

where

$$A_{mn} = \sum_{i=0}^{\alpha} (-1)^{m+i-n} a_{i,m-n+i} \frac{(m+i)!}{n!}, \qquad n \le m,$$
$$= \sum_{i=0}^{\beta} (-1)^i a_{n-m+i,i} \frac{(n-m+i)!}{n!}, \qquad n \ge m. \tag{2.9}$$

We now switch to vector notation:

$$P(t) = (P_0(t), P_1(t), \cdots), \qquad f = (f_0, f_1, \cdots), \qquad A = (A_{m,n})_{m=0,n=0}^{\infty,\infty}, \tag{2.10}$$

and then we can write our equations as

$$P'(t) = AP(t), \qquad P(0) = f. \tag{2.11}$$

Note: $A_{m,n} = 0$ unless $-\beta \le m - n \le \alpha$. Such matrices are called strip matrices.

Theorem 2.1: If f_m and A_{mn} are complex numbers such that

$$A_{mn} = 0 \quad \text{if} \quad n > m + \alpha \quad \text{for some} \quad \alpha \ge 0, \tag{2.12}$$

then problem (2.7) has a solution where each $P_m(t)$ is a formal power series in t.

Remark: By a formal power series we mean an expression of the form

$$g(t) = \sum_{n=0}^{\infty} \frac{g_n t^n}{n!}, \qquad g_n \text{ a complex number}, \tag{2.13}$$

where the series may or may not converge. Thus we first show that we have a formal power series solution and later remark on the problem of its convergence. A matrix satisfying (2.12) is called semilower diagonal.

Lemma 2.1: Let A and B be infinite matrices, i.e., $A = (A_{mn})$, $B = (B_{m,n})$, where $A_{mn} = 0$ if $n > m + \alpha$, $B_{mn} = 0$ if $n > m + \beta$. If

$$C = AB = (C_{mn}), \qquad C_{mn} = \sum_{k=0}^{\infty} A_{mk} B_{kn},$$

then

$$C_{mn} = \sum_{k=\max(n-\beta,0)}^{m+\alpha} A_{mk} B_{kn}$$

and $C_{mn} = 0$ if $n > m + \alpha + \beta$.

Proof: Clear.

Proof of Theorem 2.1: From Lemma 2.1 we see that $A^k = A^{k-1}A$ exists, and if $A^k = (A^k_{mn})$, then $A^k_{mn} = 0$ if $n > m + k\alpha$. Also, then

$$A^k f = \sum_{n=0}^{\infty} A^k_{mn} f_n = \sum_{n=0}^{m+k\alpha} A^k_{mn} f_n$$

exists. The desired solution is then given by

$$F(t) = \sum_{k=0}^{\infty} \frac{t^k}{k!} A^k f = e^{At} f. \tag{2.14}$$

Remark: For problems of convergence we refer the reader to Ref. 6, where, in particular, it is shown that if

$$L\left(x, \frac{d}{dx}\right) = a\frac{d^2}{dx^2} + bx\frac{d}{dx} + cx^2, \qquad a, b, c \text{ constants},$$

then the formal series solution for problem (2.5), in fact, converges.

Remark: The moment equations are given by a strip matrix, that is, $A_{m,n} = 0$ if $|m - n| > \beta$. In this case, the computation of A^k is greatly simplified. Moreover, if one wishes to compute the first $(j-1)$ terms of $P_0(t)$ exactly, one may truncate A to a square matrix A_1 of $(j\alpha)^2$ elements. One can then truncate A^k to a square matrix A_k of $[(j-k)\alpha]^2$, where

$$A_k = AA_{k-1},$$

where A has been truncated to $[(j-k+1)\alpha]^2$ elements and (AA_{k-1}) has been truncated to $[(j-k)\alpha]^2$ elements. Similar results hold for $P_m, m \ne 0$.

3. GORDON'S EQUATION

Consider an equation of the form

$$\frac{du}{dt} = Au, \qquad u(0) = u_0, \qquad A = L(x, D),$$

where $L(x, \xi)$ is a polynomial in 2γ variables $x = (x_1, \ldots, x_\gamma)$, $\xi = (\xi_1, \ldots, \xi_\gamma)$. We use the standard multi-index notation $n = (n_1, \ldots, n_\gamma)$, n_i is a nonnegative integer, $x^n = x_1^{n_1} \cdots x_\gamma^{n_\gamma}$, $D^n = (\partial/\partial x_1)^{n_1} \cdots (\partial/\partial x_\gamma)^{n_\gamma}$, $n! = (n_1)! \cdots (n_\gamma)!$, and $|n| = n_1 + \cdots + n_\gamma$.

If in Sec. 2 we interpret n, m, k, i, j as multi-indices, then everything is correct; in particular,

$$P_m(t) = \langle u(t), x^m \rangle = \int u(x_1, \cdots, x_\gamma, t) x_1^{m_1} \cdots x_\gamma^{m_\gamma} dx_1 \cdots dx_\gamma.$$

If $A = (A_{mn})$, $B = (B_{mn})$ are infinite matrices (or tensors), then

$$AB = \left(\sum_k A_{mk} B_{k,n}\right) = \left(\sum_{k_1=0,\ldots,k_\gamma=0}^{\infty} A_{(m_1,\ldots,m_\gamma,k_1,\ldots,k_\gamma)} B_{(k_1,\ldots,k_\gamma,n_1,\ldots,n_\gamma)}\right)$$

and so forth.

We will not write out Gordon's equation here, but we remark that is is given by a polynomial $L(x, \xi)$ in 12 ($\gamma = 6$) variables $(\beta, \beta^*, M, M^*, N_1, N_2, \xi_1, \ldots, \xi_6)$ of

degree 3. If we write $n \leq m$ for $n_1 \leq m_1, \ldots, n_\gamma \leq m_\gamma$, then

$$P(x, \xi) = \sum_{ij} a_{ij} x^i \xi^j, \quad i \leq (1,1,1,1,1,1), |i| \leq 2,$$
$$j \leq (1,1,1,1,1,1), |j| \leq 2.$$

In fact, in the moment equations

$$|n_i - m_i| \leq 1 \quad \text{or} \quad A_{m,n} = 0,$$

so that the matrix $A_{m,n}$ is a strip matrix and, consequently, the computations of the moments are relatively easy.

The question of the convergence of the formal power series solution to either the original equation or the moment equations is still open and cannot be answered by the results in Refs. 3 and 6.

4. A SIMPLE EXAMPLE

We present the following example to illustrate some of the convergence problems that we have mentioned. The equation we want to study is

$$\frac{\partial P}{\partial t} = \frac{\partial^2}{\partial x \partial y}(xyP) = LP, \quad P = P(x, y, t), \quad P(x, y, 0) = f(x, y). \tag{4.1}$$

If Gordon's equation is transformed by adiabatically eliminating the atomic polarization variables, the off diagonal diffusion terms of the resulting equation have a form similar to the right hand side of Eq. (4.1) [see Ref. 1, p. 755, Eq. (10).]

If we assume that f is analytic near zero, then

$$f(x, y) = \sum a_{mn} x^m y^n. \tag{4.2}$$

Now,

$$e^{Lt} x^m y^n = e^{(m+1)(n+1)t} x^m y^n \tag{4.3}$$

and, consequently,

$$P(x, y, t) = \sum a_{mn} e^{(m+1)(n+1)t} x^m y^n. \tag{4.4}$$

If P is to be analytic for x, y, t near 0, then

$$|a_{mn}| \leq C e^{-(m+1)(n+1)t} r^{-m-n}, \quad r \text{ small}. \tag{4.5}$$

This is a severe restriction on $f(x, y)$, in fact, if we try to choose

$$f(x, y) = e^{-x^2 - y^2} = \sum\sum \frac{(-1)^{i+j}}{(i+j)!} x^{2i} y^{2j}, \tag{4.6}$$

then we have

$$a_{nn} = 0 \quad \text{if } n \text{ is odd}$$
$$= (-1)n/n! \quad \text{if } n \text{ is even}. \tag{4.7}$$

In order to have the series (4.4) converge, we must have

$$1/n! \leq C e^{-(n+1)^2 t} r^{-2n}, \tag{4.8}$$

which is clearly impossible. Thus, the power series solution to (4.1) with f given by (4.6) does not converge, although f does have finite moments.

On the other hand, the moment equations are given by

$$P'_{pq}(t) = pg\, P_{pq}, \quad P_{pq}(0) = f_{pq}, \tag{4.9}$$

which is a diagonal system whose solution is given by

$$P_{pq}(t) = e^{pqt} f_{pq}.$$

This solution is clearly valid for any initial data f_{pq}, in marked contrast to the severe restrictions we had to place on the initial data to get analytic solutions of the previous equation. More examples are given in Ref. 9.

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*This work done in part under N.S.F. Grant No. GP 19614

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The renormalized projection operator technique for linear stochastic differential equations

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(Received 24 April 1972; revised manuscript received 3 October 1972)

A method for deriving an approximation to the equation $[\mathbb{L}_0(\mathbf{r},t)+\mathbb{L}_1(\mathbf{r},t,\omega)]\Psi(\mathbf{r},t,\omega)=g(\mathbf{r},t)$ is discussed. Two criteria for the truncation of the series are shown. The nearest neighbor equation is derived via a diagram method and the Kraichnan equation is derived.

1. INTRODUCTION

Many areas in mathematical and theoretical physics[1-4] have to deal with the solutions of linear stochastic equations. They appear in electromagnetic scattering in random media, mass and heat transport in a turbuleht fluid, in the area of solid state physics dealing with energy levels of amorphous materials plus a host of other phenomena.

The methods for solving such random equations have dealt with approximations to the well-known Neumann series and the finite approximation (or closure) of the hierarchy equations. In this paper we present a new method for solving a certain class of stochastic differential equations which is a telescoping of the first renormalization approximation. We derive two conditions for the convergence of the series and demonstrate how the nearest neighbor approximation along with the Kraichnan equation evolves; and show in the limit how these two equations approach the first renormalized approximation. The use of a diagrammatic representation is invoked to show the particular form of the nearest neighbor operator.

In Secs. 2 and 3 we briefly review the perturbation approach and the hierarchy equations and in the fourth section the renormalized projection operator technique is developed.

2. PERTURBATION APPROACH

Let us consider that the linear operator $\mathcal{L}_\omega$ can be decomposed into two parts, one of which is independent of random variations but a function of space and time, i.e., a deterministic operator $\mathbb{L}_0(\mathbf{r},t)$ and the other a random operator $\mathbb{L}_1(\mathbf{r},t,\omega)$ dependent not only on space and time but on a parameter ω which spans over a measure space or set Ω. The probability density defined over Ω is designated as $P(\omega)$. Consequently, $\mathcal{L}_\omega=\mathbb{L}_0(\mathbf{r},t)+\mathbb{L}_1(\mathbf{r},t,\omega)$ is a stochastic operator and one is considering the following stochastic equation:

$$[\mathbb{L}_0(\mathbf{r},t)+\mathbb{L}_1(\mathbf{r},t,\omega)]\Psi(\mathbf{r},t,\omega)=g(\mathbf{r},t), \tag{2.1}$$

where $g(\mathbf{r},t)$ is considered to be a nonrandom element of a linear space. $g(\mathbf{r},t)$ physically has the meaning of some source and/or sink terms and is assumed to be statistically independent of the random variable ω. If it is dependent on ω then the fluctuations in the convective process in the transport was dependent on some source and/or sink terms and vice versa. For mathematical simplicity we shall assume that this process is negligible and for a large class of physical problems this is a good assumption. We shall also assume that for a particular ω we have a unique solution of $\Psi(\mathbf{r},t)$ which is designated as $\Psi(\mathbf{r},t,\omega)$. Consequently $\Psi(\mathbf{r},t,\omega)$ is a random solution and $P(\omega)$ determines the probability density of $\Psi(\mathbf{r},t,\omega)$. The statistical measure of $\Psi(\mathbf{r},t,\omega)$, which is of interest to us is specified to be the expectation $\langle\Psi(\mathbf{r},t)\rangle=\int_\Omega\Psi(\mathbf{r},t,\omega)P(\omega)d\omega$

Equation (2.1) can be treated as a set of deterministic equations, i.e., one solves for $\Psi(\mathbf{r},t,\omega)$ for a given ω and thereby generates the set $\{\Psi(\mathbf{r},t,\omega):\omega\}$, then in order to obtain the expectation value of $\langle\Psi(\mathbf{r},t)\rangle$ one needs to know the probability density. However, such an approach is highly impractical and nearly impossible to achieve due to two reasons: (1) There is little knowledge about the probability density $P(\omega)$ and (2) it is highly unlikely to analytically solve for $\Psi(\mathbf{r},t)$ for a given ω because of boundary and initial conditions. In many physical cases this has to be done numerically; consequently, an astronomical amount of computation would have to be done to generate the set $\{\Psi(\mathbf{r},t,\omega):\omega\}$.

The parameter ϵ is a measure of departure of the operator from the deterministic operator $\mathbb{L}_0(\mathbf{r},t)$, when ϵ is a small quantity perturbation techniques can be utilized to their fullest extent.

Let us designate the solution of the deterministic part as

$$\mathbb{L}_0(\mathbf{r},t)\Psi_0^{(H)}(\mathbf{r},t)=0. \tag{2.2}$$

The operator $\mathbb{L}_1(\mathbf{r},t,\omega)$ shall be designated as a product of two operators one stochastic and the other deterministic; namely, $\delta v(\vec{x},t,\omega)\Delta(\mathbf{r},t)$. Suppose for simplicity that $\langle\mathbb{L}_1(\mathbf{r},t)\rangle=0$ implies that $\langle\delta v(\mathbf{r},t)\rangle=0$, and if $\epsilon=0$, the solution of the resulting deterministic equation $\mathbb{L}_0(\mathbf{r},t)\Psi_0^{(I)}(\mathbf{r},t)=g(\mathbf{r},t)$ is $\Psi_0^{(H)}(\mathbf{r},t)+\mathbb{L}_0^{-1}(\mathbf{r},t)g(\mathbf{r},t)$. Here $\Psi_0^{(I)}(\mathbf{r},t)$ is the inhomogeneous solution. Assuming that $\mathbb{L}_0^{-1}(\mathbf{r},t)$ exists and using the Neuman series expansion we have

$$\Psi(\mathbf{r},t,\omega)=\Psi_0^{(H)}(\mathbf{r},t)+\mathbb{L}_0^{-1}(\mathbf{r},t)g(\mathbf{r},t)-\epsilon\mathbb{L}_0^{-1}(\mathbf{r},t)\mathbb{L}_1(\mathbf{r},t,\omega)\Psi(\mathbf{r},t,\omega). \tag{2.3}$$

Now averaging to obtain $\langle\Psi(\mathbf{r},t)\rangle$, the quantity $\langle\delta v(\mathbf{r},t)\Delta(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$ must be evaluated, and, if commutativity in the operators $\delta v(\mathbf{r},t,\omega)$ and $\Delta(\mathbf{r},t)$ exist, then $\Delta(\mathbf{r},t)\langle\delta v(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$.

Expanding the series in terms of the unperturbed solution one arrives at

$$\Psi(\mathbf{r},t,\omega)=[1-\epsilon\mathbb{L}_0^{-1}(\mathbf{r},t)\mathbb{L}_1(\mathbf{r},t,\omega)+\epsilon^2\mathbb{L}_0^{-1}(\mathbf{r},t)\mathbb{L}_1(\mathbf{r},t,\omega)\mathbb{L}_0^{-1}(\mathbf{r},t)\mathbb{L}_1(\mathbf{r},t,\omega)+\mathcal{O}(\epsilon^3)\cdots][\Psi_0^H(\mathbf{r},t)+\mathbb{L}_0^{-1}(\mathbf{r},t)g(\mathbf{r},t)]. \tag{2.4}$$

Taking the expectation values, and retaining terms to $\mathcal{O}(\epsilon^2)$ we have

$$\langle\Psi(\mathbf{r},t)\rangle = \Psi_0^H(\mathbf{r},t) + \mathrm{L}_0(\mathbf{r},t)g(\mathbf{r},t) + \epsilon^2\mathrm{L}_0^{-1}(\mathbf{r},t)\langle\delta v(\mathbf{r},t)\Delta(\mathbf{r},t) \times \mathrm{L}_0^{-1}(\mathbf{r},t)\delta v(\mathbf{r},t)\Delta(\mathbf{r},t)\rangle[\Psi_0^H(\mathbf{r},t) + \mathrm{L}_0^{-1}(\mathbf{r},t)g(\mathbf{r},t)]. \quad (2.5)$$

Equivalently, since

$$\Psi_0^H(\mathbf{r},t) + \mathrm{L}_0^{-1}(\mathbf{r},t)g(\mathbf{r},t) = \langle\Psi(\mathbf{r},t)\rangle + \Theta(\epsilon^2) \quad (2.6)$$

we have

$$[\mathrm{L}_0(\mathbf{r},t) - \epsilon^2\langle\delta v(\mathbf{r},t)\Delta(\mathbf{r},t)\mathrm{L}_0^{-1}(\mathbf{r},t) \times \delta v(\mathbf{r},t)\Delta(\mathbf{r},t)\rangle]\langle\Psi(\mathbf{r},t)\rangle = g(\mathbf{r},t). \quad (2.7)$$

The question now arises, what is the inverse operator of $\mathrm{L}_0(\mathbf{r},t)$.

It is an n-order matrix which we shall represent as an integral operator. Namely, consider the equation

$$\mathrm{L}_0(\mathbf{r},t)G(\mathbf{r},t|\mathbf{r}',t') = 1\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'), \quad (2.8)$$

where 1 is the unit matrix and δ is the Dirac delta. Now in general

$$\mathrm{L}_0^{-1}(\mathbf{r},t)\delta v(\mathbf{r},t,\omega)\Delta(\mathbf{r},t) = \iint d\mathbf{r}'dt'G(\mathbf{r},t|\mathbf{r}',t')\delta v(\mathbf{r}',t',\omega)\Delta(\mathbf{r}',t'). \quad (2.9)$$

The kernel $G(\mathbf{r},t|\mathbf{r}',t')$ is the Green matrix and is defined by Eq. (2.8) utilizing the fact that the inverse operator has an integral operator representation. Equation (2.7) becomes

$$\mathrm{L}_0(\mathbf{r},t)\langle\Psi(\mathbf{r},t)\rangle - \epsilon^2\iint d\mathbf{r}'dt'\Delta(\mathbf{r},t)\langle\delta v(\mathbf{r},t) \times \delta v(\mathbf{r}',t')\rangle G(\mathbf{r},t|\mathbf{r}',t') \times \Delta(\mathbf{r}',t')\langle\Psi(\mathbf{r}',t')\rangle = g(\mathbf{r},t). \quad (2.10)$$

Equation (2.10) is a very well-known stochastic equation [cf. Adomian[5,6] and Keller[7]]. In the case when $\mathrm{L}_0^{-1}(\mathbf{r},t)$ is some differential operator, one has a linear integrodifferential equation to solve. In the case when the average $\langle\Psi(\mathbf{r},t)\rangle$ in the integrand is replaced by $\Psi_0^H(\mathbf{r},t) + \iint d\mathbf{r}''dt''G(\mathbf{r},t|\mathbf{r}'',t'')g(\mathbf{r}''t'')$, the equation becomes an inhomogeneous differential equation and is equivalent to the first Born approximation.

A number of approximations are inherent in the integrodifferential equation; namely, (1) all the information concerning the randomness is contained in the two point correlation function, and (2) the operator

$$[\mathrm{L}_0(\mathbf{r},t) + \langle\mathrm{L}_1(\mathbf{r},t)\mathrm{L}_0^{-1}(\mathbf{r},t)\mathrm{L}_1(\mathbf{r},t)\rangle]^{-1}$$

which is related to the stochastic Green function, can easily be shown to be equivalent to the infinite series:

$$\sum_{m=0}^{\infty}(-1)^m[\mathrm{L}_0^{-1}(\mathbf{r},t)\langle\mathrm{L}_1(\mathbf{r},t)\mathrm{L}_0^{-1}(\mathbf{r},t)\mathrm{L}_1(\mathbf{r},t)\rangle]^m\mathrm{L}_0(\mathbf{r},t).$$

Consequently this operator is a sum of a subset of infinite number of terms of the "averaged" perturbation series.

A third approximation is the effect that the boundary conditions have on the fluctuations have been ignored.

Thus, one can see that when the fluctuations are small one may only need calculate a few terms in the series in order to approximate the true averate of $\langle\Psi(\mathbf{r},t)\rangle$. In the above we summed an infinite number of terms in the series. This is termed, "a renormalization technique"; and under some cases convergence can be guaranteed and the problem of secularity can be avoided.

3. HIERARCHY EQUATIONS

In solving the stochastic Eq. (2.1) the hierarchical approach has received considerable attention in recent years. The reader is referred to the notable works of Kraichnan[8-10] and Roberts.[11,12] This procedure involves the generation of a hierarchy of equations and using some truncation process to determine the hierarchy. Now if the averaging process is immediately applied to equation (2.1) we obtain

$$\mathrm{L}_0(\mathbf{r},t)\langle\Psi(\mathbf{r},t)\rangle + \langle\mathrm{L}_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle = g(\mathbf{r},t). \quad (3.1)$$

In the second term on the left-hand side, the operator $\mathrm{L}_1(\mathbf{r},t,\omega)$ and $\Psi(\mathbf{r},t,\omega)$ are not statistically independent and cannot be separated for the evaluation of the expected value $\langle\Psi(\mathbf{r},t)\rangle$. Since we wish to determine $\langle\mathrm{L}_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$, we multiply Eq. (2.1) by $\mathrm{L}_1(\mathbf{r},t,\omega)$ and perform the averaging again, and obtain the term $\langle\mathrm{L}_1(\mathbf{r},t)\mathrm{L}_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$. However, we do not in general have commutativity between $\mathrm{L}_0(\mathbf{r},t)$ and $\mathrm{L}_1(\mathbf{r},t,\omega)$, i.e., $[\mathrm{L}_0(\mathbf{r},t), \mathrm{L}_1(\mathbf{r},t,\omega)] \neq 0$, but for the present we shall assume that the condition $[\mathrm{L}_0(\mathbf{r},t), \delta v(\mathbf{r},t,\omega)] = 0$; therefore, if we multiply by $\mathrm{L}_1(\mathbf{r}_1,t_1,\omega)$ and average we arrive at

$$\mathrm{L}_0(\mathbf{r},t)\langle\mathrm{L}_1(\mathbf{r}_1,t_1)\Psi(\mathbf{r},t)\rangle + \langle\mathrm{L}_1(\mathbf{r},t)\mathrm{L}_1(\mathbf{r}_1,t_1)\Psi(\mathbf{r},t)\rangle = \langle\mathrm{L}_1(\mathbf{r}_1,t_1)\rangle g(\mathbf{r},t). \quad (3.2)$$

If we could solve for the first term and evaluate the results in the limit $\mathbf{r}_1 \to \mathbf{r}$ and $t_1 \to t$ and upon substitution back, we would obtain the average value of the average of the scalar function $\langle\Psi(\mathbf{r},t)\rangle$. Aside from the generally ignored question of the validity of the above limit, one observes that we now need a new moment $\langle\mathrm{L}_1(\mathbf{r}_1,t_1)\mathrm{L}_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$; consequently, it is necessary to repeat the procedure, and by multiplying we are led to an infinite set of equations called the hierarchy equations for the hierarchy of moments. If we desire also the higher moments of $\Psi(\mathbf{r},t)$, one proceeds in the same manner multiplying by $\Psi(\mathbf{r}_1,t_1)$. Thus the solution which has been justified only by its arbitrary assumption.

If, at any level in the hierarchical scheme, the closure approximation can be made then the hierarchy can be terminated. Thus, if

$$\langle\mathrm{L}_1(\mathbf{r}_1,t_1)\mathrm{L}_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle = \langle\mathrm{L}_1(\mathbf{r}_1,t_1)\mathrm{L}_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle \quad (3.3)$$

in Eq. (3.2), we can solve for the cross correlation function at $\mathbf{r}_1 \to \mathbf{r}$ and $t_1 \to t$ and substitute into Eq. 3.1 to solve for $\langle\Psi(\mathbf{r},t)\rangle$. This is under the assumption that $\mathrm{L}_0(\mathbf{r},t)$ is a known operator and the initial conditions are specified. One other possibility exists, but appears to be of little physical interest. If there exists a very small correlation length for $\mathrm{L}_1(\mathbf{r},t)$ compared to $\Psi(\mathbf{r},t)$, i.e., if $\delta v(\mathbf{r},t,\omega)$ is varying rapidly compared to $\Psi(\mathbf{r},t,\omega)$, the truncation can be justified.

The same method (hierarchical scheme) has been used to obtain a correlation function for $\Psi(\mathbf{r},t,\omega)$ or its higher moments, the general case gives an infinite set of equations:

$$\begin{aligned}&L_0(\mathbf{r},t)\langle\Psi(\mathbf{r},t)\Psi(\mathbf{r}_1,t_1)\cdots\Psi(\mathbf{r}_j,t_j)\\&\quad\times L_1(\mathbf{r}_{j+1},t_{j+1})\cdots L_1(\mathbf{r}_{j+k},t_{j+k})\rangle\\&\quad+\langle L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\Psi(\mathbf{r}_1,t_1)\cdots\Psi(\mathbf{r}_j,t_j)\\&\quad\times L_1(\mathbf{r}_{j+1},t_{j+1})\cdots L_1(\mathbf{r}_{j+k},t_{j+k})\rangle\\&=g(\mathbf{r},t)\langle\Psi(\mathbf{r}_1,t_1)\cdots\Psi(\mathbf{r}_j,t_j)\cdots L_1(\mathbf{r}_{j+k},t_{j+k})\rangle.\end{aligned}\tag{3.4}$$

Since the source term $g(\mathbf{r},t)$ is assumed to be statistically independent of the fluctuations, we see that an infinite set of equations are needed to find all moments, i.e., any moment involves all the moments of higher order and the closure procedure is necessary to obtain a cutoff. Thus, in the kth member of the hierarchy we set

$$\begin{aligned}&\langle L_1(\mathbf{r}_1,t_1)\cdots L_1(\mathbf{r}_{k-1},t_{k-1})L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle\\&\quad\simeq\langle L_1(\mathbf{r}_1,t_1)\cdots L_1(\mathbf{r}_{k-1},t_{k-1})L_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle.\end{aligned}\tag{3.5}$$

Adomian[2] showed the relationship between the hierarchical approach and the perturbation approach. Previously we have stated that the expectation of Eq. (3.1) is

$$L_0(\mathbf{r},t)\langle\Psi(\mathbf{r},t)\rangle+\epsilon\langle L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle=g(\mathbf{r},t).\tag{3.6}$$

Since $\langle L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$ is unknown and cannot be separated without perturbation theory, we solve Eq. (3.1) for $\Psi(\mathbf{r},t,\omega)$ by multiplying by $L_0^{-1}(\mathbf{r},t)$ and obtain

$$\Psi(\mathbf{r},t,\omega)+\epsilon L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t,\omega)\Psi(\mathbf{r},t,\omega)=L_0^{-1}(\mathbf{r},t)g(\mathbf{r},t).\tag{3.7}$$

Now, if we multiply Eq. (3.7) by $L_1(\mathbf{r},t,\omega)$ and obtain the average, we have

$$\langle L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle+\epsilon\langle L_1(\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle.\tag{3.8}$$

To avoid further complications, we assume "blindly" (the closure approximation or the so-called local independence) that

$$\begin{aligned}&\langle L_1(\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle\\&\qquad\simeq\langle L_1(\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle.\end{aligned}\tag{3.9}$$

Now,

$$\langle L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle\simeq-\epsilon\langle L_1(\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle.\tag{3.10}$$

Substituting Eq. (3.10) into Eq. (3.6), we obtain

$$L_0(\mathbf{r},t)\langle\Psi(\mathbf{r},t)\rangle-\epsilon^2\langle\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle=g(\mathbf{r},t).\tag{3.11}$$

This is the same result that was obtained from perturbation theory, as Keller[7] points out, when the randomness is small, i.e., when the perturbation approach is useful, the average $\langle L_1(\mathbf{r}_1,t_1)L_0(\mathbf{r},t)L_1(\mathbf{r},t)\Psi(\mathbf{r},t)\rangle$ can be written $\langle L_1(\mathbf{r},t)L_0^{-1}(\mathbf{r},t)L_1(\mathbf{r},t)\rangle\langle\Psi(\mathbf{r},t)\rangle$.

If $\mathcal{L}_\omega$ is a differential operator, it is obviously wrong to assume statistical independence of $\mathcal{L}_\omega$ and its operand $\Psi(\mathbf{r},t,\omega)$, although we have previously said it is reasonable to assume statistical independence of $\mathcal{L}_\omega$ and $g(\mathbf{r},t)$, i.e., $\langle\mathcal{L}_\omega(\mathbf{r},t)\rangle=\langle\mathcal{L}_\omega\rangle\langle g(\mathbf{r},t)\rangle$.

The hierarchy method has had wide use in statistical physics. In the theory of turbulence, the dynamical equations lead to an infinite hierarchy of coupled equations where the given ensemble averages are related to successively higher order terms. This difficulty occurs in the linear case as well. The closure approximations (a truncation and closure of the hierarchy) is always assumed to find an approximation for the desired statistical quantities, but the validity or error has not been adequately discussed.

Turbulent convection which occurs in nature governs the transport of heat and mass. A general feature of a theory of turbulence is a infinite set of dynamical equations which couple together all the moments of a statistical distribution of the velocity field. The closure problem associated with this problem as Kraichnan points out is: How are they replaced by a finite set that yields the limited statistical information of actual interest? In the hierarchical approach to this problem closure becomes a glaring problem.

4. THE RENORMALIZED-PROJECTED APPROACH

In the case of strong turbulent convective processes, perturbation theory breaks down and the closure problem becomes evident in the hierarchical scheme. In this approach we utilize some projection operator that telescopes a "low" order renormalization process. From the derived equation we can show a strict condition for convergence of the series which is related to the closure approximation in the hierarchical scheme.

In this method the scalar or vector function $\Psi(\mathbf{r},t)$ can be written as

$$\Psi(\mathbf{r},t,\omega)=[1-(L_0-\langle L_1L_0^{-1}L_1\rangle^{-1}\langle\mathbb{P}\rangle]\langle\Phi(\mathbf{r},t)\rangle+\delta\Psi(\mathbf{r},t,\omega),\tag{4.1}$$

where $\delta\Psi(\mathbf{r},t,\omega)$ is the random fluctuation in the field. The expected value of the field is $\langle\Psi(\mathbf{r},t)\rangle=[1-(L_0-\langle L_1L_0^{-1}L_1\rangle)^{-1}\langle\mathbb{P}\rangle]\langle\Phi(\mathbf{r},t)\rangle$. [The expected value of the operator $\langle\mathbb{P}(\mathbf{r},t)\rangle$ will be shown to be any subset of strongly connected graphs.] Also we assume that the average of the fluctuations is zero. Again we are considering the stochastic equation

$$[L_0(\mathbf{r},t)+L_1(\mathbf{r},t,\omega)]\Psi(\mathbf{r},t,\omega)=g(\mathbf{r},t).\tag{4.2}$$

If we substitute Eq. (4.1) into Eq. (4.2) and average, we obtain

$$\begin{aligned}&L_0[1-(L_0-\langle L_1L_0^{-1}L_1\rangle^{-1}\langle\mathbb{P}\rangle]\langle\phi(\mathbf{r},t)\rangle\\&\qquad=\langle L_1\delta\Psi(\mathbf{r},t)\rangle+g(\mathbf{r},t);\end{aligned}\tag{4.3}$$

again we are confronted with evaluation of $\langle L_1\delta\Psi(\mathbf{r},t)\rangle$.

$\mathbb{P}(\mathbf{r},t,\omega)$ is a projection of the average value for the scalar or vector function

If we subtract Eqs. (4.3) and (4.2), we obtain

$$\begin{aligned}\delta\Psi(\mathbf{r},t,\omega)=\;&L_0^{-1}(L_1\delta\Psi(\mathbf{r},t,\omega)-\langle L_1\delta\Psi(\mathbf{r},t)\rangle)\\&+L_0^{-1}L_1[1-(L_0-\langle L_1L_0^{-1}L_1\rangle)^{-1}\\&\times\langle\mathbb{P}\rangle]\langle\phi(\mathbf{r},t)\rangle.\end{aligned}\tag{4.4}$$

Following along the lines of Tararski,[13-15] we shall

define the operator $\hat{G}$ to be

$$\hat{G} = G - \langle G \rangle \tag{4.5}$$

and the operator $\Omega(\mathbf{r}, t)$ to be

$$\Omega\Psi(\mathbf{r}, t, \omega) \equiv L_0^{-1} \widehat{L_1\Psi(\mathbf{r}, t, \omega)} = L_0^{-1}(L_1\Psi(\mathbf{r}, t, \omega) - \langle L_1\Psi(\mathbf{r}, t)\rangle). \tag{4.6}$$

Thus, we have

$$\Omega\langle\Psi(\mathbf{r}, t)\rangle = L_0^{-1}L_1[1 - (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle]\langle\phi(\mathbf{r}, t)\rangle \tag{4.7}$$

and, also,

$$\Omega\delta\Psi(\mathbf{r}, t, \omega) = L_0^{-1}(L_1\delta\Psi(\mathbf{r}, t, \omega) - \langle L_1\delta\Psi(\mathbf{r}, t)\rangle). \tag{4.8}$$

This operator is employed because of its important property: $\langle\Omega^n\Psi(\mathbf{r}, t)\rangle = 0$ for any function $\Psi(\mathbf{r}, t, \omega)$ and for any n. Indeed,

$$\langle\Omega\Omega^{N-1}\Psi(\mathbf{r}, t)\rangle = \langle L_0^{-1}\widehat{L_1\Omega^{N-1}\Psi(\mathbf{r}, t)}\rangle = L_0^{-1}(\langle L_1\Omega^{N-1}\Psi(\mathbf{r}, t)\rangle - \langle\langle L_1\Omega^{N-1}\Psi(\mathbf{r}, t)\rangle\rangle) = 0. \tag{4.9}$$

Utilizing the above equation, the cross correlation functions become

$$\langle L_1\delta\Psi(\mathbf{r}, t)\rangle = \langle L_1\Omega\delta\Psi(\mathbf{r}, t)\rangle + \langle L_1\Omega\rangle[1 - (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle]\langle\phi(\mathbf{r}, t)\rangle, \tag{4.10}$$

since

$$(L_0 - \langle L_1\Omega\rangle)(1 - (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle) = L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle. \tag{4.11}$$

Consequently, the equation for the mean value of $\langle\phi(\mathbf{r}, t)\rangle$ and the fluctuation $\delta\Psi(\mathbf{r}, t, \omega)$ becomes

$$\langle\phi(\mathbf{r}, t)\rangle = (L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle)^{-1}[g(\mathbf{r}, t) - \langle L_1\Omega\delta\Psi(\mathbf{r}, t)\rangle] \tag{4.12}$$

and

$$\delta\Psi(\mathbf{r}, t, \omega) = \Omega\delta\Psi(\mathbf{r}, t, \omega) + \Omega\langle\phi(\mathbf{r}, t)\rangle - \Omega(L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1} \times \langle\mathbb{P}\rangle\langle\phi(\mathbf{r}, t)\rangle. \tag{4.13}$$

This set of equations can be consecutively solved to yield

$$\langle\phi(\mathbf{r}, t)\rangle = (L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle)^{-1}\{g(\mathbf{r}, t) - \langle L_1\Omega^2\delta\Psi(\mathbf{r}, t)\rangle + \langle L_1\Omega^2\rangle[1 - (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle] \times [L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle] \times [g(\mathbf{r}, t) + \langle L_1\Omega\delta\Psi(\mathbf{r}, t)\rangle] + \cdots\}, \tag{4.14}$$

$$\delta\Psi(\mathbf{r}, t, \omega) = \Omega\delta\Psi(\mathbf{r}, t, \omega) + \Omega[1 - (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle] \times [L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle]^{-1}[g(\mathbf{r}, t) + \langle L_1\Omega\delta\Psi(\mathbf{r}, t)\rangle] + \cdots \tag{4.15}$$

$$\langle\phi(\mathbf{r}, t)\rangle = [L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle]^{-1}\{g(\mathbf{r}, t) + \langle L_1\Omega^2\rangle \times [1 + (L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle] \times [L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle]^{-1} \times g(\mathbf{r}, t) + \cdots\}. \tag{4.16}$$

The interesting feature of this procedure is that, unlike the "normal" perturbation series in Eq. (2.4), we have generated a series in powers of the operator $[L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle]^{-1}$. This in itself can be expanded in an infinite series

$$[L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle]^{-1} = \sum_{z=0}^{\infty}\left(\sum_{k=0}^{\infty}(L_0\langle L_1 L_0^{-1} L_1\rangle)^k L_0^{-1}\langle\mathbb{P}\rangle\right) \times \sum_{k'=0}^{\infty}(L_0\langle L_1 L_0 L_1\rangle)^{k'} L_0^{-1}. \tag{4.17}$$

Thus, the above operator is a sum of an infinite number of terms, and taking the limit as $\langle\mathbb{P}\rangle \to 0$, Eq. (4.17) approaches $\sum_{k=0}^{\infty}(L_0\langle L_1 L_0^{-1} L_1\rangle)^k L_0$.

Since we can write the kernel of the operator $(L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle)^{-1}$ in analytic form, each term of Eq. (4.16) is already a sum of an infinite number of components taken from the perturbation series or the first approximation in the hierarchy equations.

If we consider the case when we have the following conditions, (1) $\|(L_0 - \langle L_1 L_0^{-1} L_1\rangle)^{-1}\langle\mathbb{P}\rangle\| \ll 1$, (2) $(L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle)^{-1}g(\mathbf{r}, t)$ is the leading term in the series (4.16), then $\langle\Psi(\mathbf{r}, t)\rangle \simeq \langle\phi(\mathbf{r}, t)\rangle$, and the solution is $\langle\phi(\mathbf{r}, t)\rangle \simeq (L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle\mathbb{P}\rangle)^{-1}g(\mathbf{r}, t)$. It is very interesting to note that if $\langle\mathbb{P}\rangle = 0$, we obtain the first renormalized equation

$$(L_0 - \langle L_1 L_0^{-1} L_1\rangle)\langle\Psi(\mathbf{r}, t)\rangle = g(\mathbf{r}, t). \tag{4.18}$$

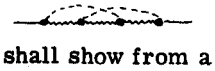
Also, if the operator $\langle\mathbb{P}\rangle \equiv -\langle L_1 L_0^{-1} L_1\rangle + \langle L_0\langle(L_0 + L_1)^{-1}\rangle L_1\rangle$, we have the Kraichnan equation

$$[L_0 - \langle L_1\langle(L_0 + L_1)^{-1}\rangle L_1\rangle]\langle\Psi(\mathbf{r}, t)\rangle = g(\mathbf{r}, t). \tag{4.19}$$

This equation is a nonlinear stochastic equation and has been shown to be very successful in the turbulent problem connected with the Navier-Stokes equation along with the turbulent diffusion equation. The operator $\langle\mathbb{P}\rangle$ is extremely crucial. We will show by using diagram techniques how one can choose a certain $\langle\mathbb{P}\rangle$ to represent a given class of diagrams. As to the question of whether this class of diagrams adequately represents the physical situation is another question. Plausibility arguments can be given as with Kraichnan or, if possible, with the help of experimental and computational means one could show what terms of the n-point correlation functions are pertinent. However, this is a very formidable task.

Another example of the operator $\langle\mathbb{P}\rangle$ is $\langle L_1 L_0^{-1} L_1 L_0^{-1} L_1 L_0^{-1} L_1\rangle$.

This corresponds to the next nearest neighbor interaction and has as its subject all graphs of the form



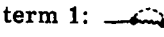
We shall show from a purely diagrammatical approach one can deduce the equation

$$[L_0 - \langle L_1 L_0^{-1} L_1\rangle - \langle L_1 L_0^{-1} L_1 L_0^{-1} L_1 L_0^{-1} L_1\rangle]\langle\Psi(\mathbf{r}, t)\rangle = g(\mathbf{r}, t). \tag{4.20}$$

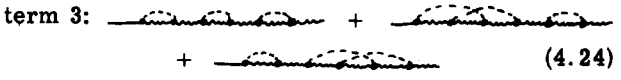
Now from the diagram technique (LoData,[3] Frish,[16]) let us derive a particular form of the renormalized operator $\langle\mathbb{P}\rangle$. Consider a process whose major inter-

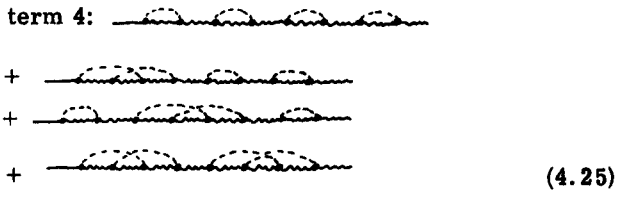
actions are of the scale $|\mathbf{r}_i - \mathbf{r}_{i+1}|, |\mathbf{r}_{i+1} - \mathbf{r}_{i+2}|, t_{i+1} - t_i$, and $t_{i+2} - t_{i+1}$. Hence, the major diagrams in the series become

term 0:  (4.21)

term 1:  (4.22)

term 2:  (4.23)

term 3:  (4.24)

term 4:  (4.25)

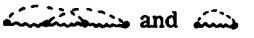
.
.
.

etc.

For the kth term ($k \geq 3$), we have $\sum_{i=1}^{[k/2]-1} (k-1-i)!/(i+1)!(k-2-2i)!$ components, and for total number of terms $T(N)$ we have

$$T_{(N)} \begin{cases} 1 & N = 1 \\ 3 & N = 2 \\ N + 1 + \sum_{m=0}^{N-3} \sum_{i=0}^{[(m+3)/2]-1} \dfrac{(m+2-i)!}{(i+1)!(m+1-2i)!} \end{cases}. \tag{4.26}$$

The terms corresponding to

 and

we shall represent as B_4 and B_2, respectively. Considering the sum of the series of all these diagrams, we shall proceed as follows: We consider the sum of the diagram with the structure of one B_4 and we see

$$\begin{aligned} &B_4 \\ &+ B_4B_2 + B_2B_4 \\ &+ B_4B_2^2 + B_2B_4B_2 + B_2^2B_4 \\ &+ B_4B_2^3 + B_2B_4B_2^2 + B_2^2B_4B_2 + B_2^3B_4 \\ &\quad\vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \end{aligned} \tag{4.27}$$

Summing down each column, we have

$$B_4(1-B_2)^{-1} + B_2B_4(1-B_2)^{-1} + B_2^2B_4(1-B_2)^{-1} + \cdots. \tag{4.28}$$

Now summing across, we see that the total number of terms contain just one B_4 type diagram can be represented as

$$(1-B_2)^{-1}B_4(1-B_2)^{-1}. \tag{4.29}$$

For the case where there are no B_4 diagrams the sum becomes $(1-B_2)^{-1}$. For the case where there are two B_4 diagrams we have the following:

$$\begin{aligned} &B_4^2 \\ &+ B_4^2B_2 + B_4B_2B_4 + B_2B_4^2 \\ &+ B_4^2B_2^2 + B_4B_2^2B_4 + B_2^2B_4^2 + B_2B_4B_2B_4 + B_4B_2B_4B_2 \\ &+ B_4^2B_2^3 + B_4B_2^3B_4B_2^3B_4^2 + B_2^2B_4B_2B_4 + B_4B_2B_4B_2^2 + B_4B_2^2B_4B_2 + \cdots. \\ &\quad\vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \quad\quad \vdots \end{aligned} \tag{4.30}$$

Again by summing down and summing across, the total number of terms contributing to two B_4 diagrams is

$$(1-B_2)^{-1}B_4(1-B_2)^{-1}B_4(1-B_2)^{-1}. \tag{4.31}$$

Now, with the summing of the B_4 diagrams we have

$$\begin{aligned} &[(1-B_2)^{-1} + (1-B_2)^{-1}B_4(1-B_2)^{-1} \\ &\quad + (1-B_2)^{-1}B_4(1-B_2)^{-1}B_4(1-B_2)^{-1} \\ &\quad + \cdots] = (1-B_2)^{-1}[1-B_4(1-B_2)^{-1}]^{-1}. \end{aligned} \tag{4.32}$$

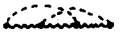
Therefore, the sum of all terms involving B_2 and B_4 type diagrams is $\{[1-B_4(1-B_2)^{-1}][1-B_2]\}^{-1}$. We shall recall that B_2 and B_4 are strong diagrams, i.e., they are not factorable and that when B_4 is zero or nonexistent we have the first bubble approximation

 .

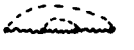
Hence, the operator representation of the sum of graphs $(1-B_2)^{-1}$ is

$$[\mathbf{L}_0 - \langle \mathbf{L}_1 \mathbf{L}_0^{-1} \mathbf{L}_1 \rangle] = (1-B_2)^{-1}, \tag{4.33}$$

and B_4 is a strong diagram in this particular case we have chosen B_4 to have the structure



However, it could have been this one



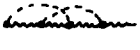
or any other one, hence we will define $B_4 = \langle \mathrm{P} \rangle$. Thus we have

$$\begin{aligned} \langle \Psi(\mathbf{r},t) \rangle = \{[1 - \langle \mathrm{P} \rangle (\mathbf{L}_0 - \langle \mathbf{L}_1 \mathbf{L}_0^{-1} \mathbf{L}_1 \rangle)^{-1}] \\ \times [\mathbf{L}_0 - \langle \mathbf{L}_2 \mathbf{L}_0^{-1} \mathbf{L}_1 \rangle]\}^{-1} g(\mathbf{r},t) \end{aligned} \tag{4.34}$$

or

$$[\mathbf{L}_0 - \langle \mathbf{L}_1 \mathbf{L}_0^{-1} \mathbf{L}_1 \rangle - \langle \mathrm{P} \rangle] \langle \Psi(\mathbf{r},t) \rangle = g(\mathbf{r},t). \tag{4.35}$$

In the particular case where the operation $\langle \mathrm{P} \rangle$ has the structure



The integro-differential equation (LoDato[3]) becomes

$$L_0(1)\langle\Psi(1)\rangle - \epsilon^2 \int d2\langle\delta v(1)\delta v(2)\rangle\Delta(1)G(1|2)\Delta(2)\langle\Psi(2)\rangle - \epsilon^4 \iiint d2d3d4\langle\delta v(1)\delta v(3)\rangle \times \langle\delta v(2)\delta v(4)\rangle\Delta(1)G(2|2)\Delta(2) \times G(2|3)\Delta(3)G(3|4)\Delta(4)\langle\Psi(4)\rangle = g(1). \quad (4.36)$$

The third term on the right-hand side corresponds to a next to nearest neighbor interaction term. To recapitulate what we said earlier: In order to choose the proper diagrams to assure convergence of the perturbation series, it has been based on physical intuition or numerical experimentation in calculating the n-point correlation function. Let us now consider the solution of the Kraichnan equation

$$[L_0 - \langle L_1\langle\mathfrak{L}^{-1}\rangle L_1\rangle]\langle\mathfrak{L}^{-1}\rangle = 1. \quad (4.37)$$

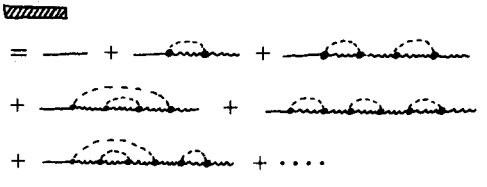
The solution of such a nonlinear equation can be written by means of a continuous fraction

$$\langle\mathfrak{L}^{-1}\rangle = [L_0 - \langle L_1\langle\mathfrak{L}^{-1}\rangle L_1\rangle]^{-1}, \quad (4.38)$$

$$\langle\mathfrak{L}^{-1}\rangle = [L_0 - \langle L_1[L_0 - \langle L_1\langle\mathfrak{L}^{-1}\rangle L_1\rangle]^{-1} L_1\rangle]^{-1}, \quad (4.39a)$$

$$\langle\mathfrak{L}^{-1}\rangle = [L_0 - \langle L_1[L_0 - \langle L_1[L_0 - \langle L_1[L_0 \cdots L_1\rangle]^{-1} L_1\rangle]^{-1} L_1\rangle]^{-1} L_1\rangle]^{-1} \quad (4.39b)$$

From a diagram representation this corresponds to the class of diagrams that are made of nonintersecting dotted lines and only two point interconnections of dotted lines. Consequently, the mean Green's function becomes



(4.40)

In the case when the perturbation is small it reduces to the first order renormalization case, and, when the process is highly turbulent, the covariance $\langle\delta v(\mathbf{r}, t)\delta v(\mathbf{r}', t')\rangle$ can be replaced by a constant and can be solved by a Fourier transformation.

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Convergence in the mean of solutions to the neutron integral Boltzmann equation in three-dimensional systems

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(Received 12 July 1972; revised manuscript received 3 October 1972)

The Neumann series solution as well as practical solutions for the stationary integral Boltzmann equation, which governs the flux distribution of monoenergetic neutrons in a three-dimensional system made by an isotropically scattering and multiplying material, are built up by extensively using the concept of double norm and the theory of bounded linear integral transformations in a Lebesgue space L_p. The convergence in the mean as well as other basic properties of the proposed solutions are studied for the cases of both distributed and isotropic deltalike sources.

1. INTRODUCTION

Methods based on either the singular eigenfunction or the Fourier transform techniques have so far been proposed for solving the steady-state linear integral and integro-differential Boltzmann equations for monoenergetic neutrons.

In a recent paper,[1] where comparison is made between the singular eigenfunction and the Fourier transform methods, Case and Hazeltine observe that "the Fourier transform method seems in several ways more direct; in particular it provides solutions directly in a form suitable for evaluation."

In this paper we propose an approach which seems to be much more direct than either of the two methods mentioned above. This approach, which particularly refers to the constructive techniques of functional analysis, allows us to build up, directly in their original domain of definition, very manageable solutions to the integral form of the monoenergetic neutron linear Boltzmann equation in the most general case of a spatially distributed source as well as for the source-free configuration of three-dimensional systems.

We consider in the three-dimensional Euclidean space R_3, a body surrounded by void and occupying a convex, finite, closed, and measurable domain D of finite measure V; let $\bar{x}$ be a point in the interior of D. A source $Q(\bar{x})$ emitting monoenergetic neutrons at a constant rate in time is distributed throughout the body: according to any realistic situation $Q(\bar{x})$ is a bounded, real, nonnegative, measurable function for $\bar{x} \in D$. The body is made of a material in which both scattering and fission are taken to be spherically symmetric in the laboratory system. For the sake of generality two further options are actually incorporated in the theory.

The first concerns the nuclear properties of the material of which the body is made: It may even be inhomogeneous, that is, its total, scattering, absorption, and fission macroscopic cross sections (to be denoted in the sequel as $\Sigma, \Sigma_s, \Sigma_a$, and Σ_f, respectively) can be functions of the point $\bar{x}' \in D$ at which neutrons are isotropically produced by scattering and fission. We set

$$\begin{aligned} \Sigma(\bar{x}') &= \Sigma_s(\bar{x}') + \Sigma_a(\bar{x}') + \Sigma_f(\bar{x}'), \\ \Sigma_{sf}(\bar{x}') &= \Sigma_s(\bar{x}') + \nu(\bar{x}')\Sigma_f(\bar{x}'), \end{aligned} \tag{1}$$

ν being the mean number of secondary neutrons per fission.

We assume that both $\Sigma(\bar{x}')$ and $\Sigma_{sf}(\bar{x}')$ are bounded real nonnegative measurable functions for $\bar{x}' \in D$ though they may exhibit a finite number of discontinuity surfaces $S_i^*(i = 1, 2, \ldots, n)$ of finite measure (for instance, they may be the surfaces separating two or more different media of which the body consists). In this connection we recall that $\Sigma(\bar{x}') = \Sigma_{sf}(\bar{x}') = 0$ when $\bar{x}'$ is a point in a void.

The second option concerns, instead, the nature of the surface S delimiting the body considered, which may even be concave. In this case it can still be regarded as occupying a convex domain D which includes the body surrounded by voids.

Our task is then to evaluate the neutron total flux $\phi_0(\bar{x})$ as defined at any $\bar{x} \in D$ by the stationary linear integral Boltzmann equation, which for the physical situation above illustrated reads as[2]

$$\phi_0(\bar{x}) = \int_D d_3x' \, \frac{e^{-\tau(\bar{x},\bar{x}')}}{4\pi|\bar{x}-\bar{x}'|^2} [\Sigma_{sf}(\bar{x}')\phi_0(\bar{x}') + Q(\bar{x}')], \tag{2}$$

where

$$\tau(\bar{x},\bar{x}') = \int_0^{|\bar{x}-\bar{x}'|} \Sigma\left(\bar{x} - \frac{\bar{x}-\bar{x}'}{|\bar{x}-\bar{x}'|}u\right) du \tag{3}$$

is the optical distance between $\bar{x}$ and $\bar{x}'$.

For the kernel of Eq. (2) we set

$$K_{sf}(\bar{x},\bar{x}') = \Sigma_{sf}(\bar{x}')K_\tau(\bar{x},\bar{x}') = \Sigma_{sf}(\bar{x}')\, e^{-\tau(\bar{x},\bar{x}')}/4\pi|\bar{x}-\bar{x}'|^2 \tag{4}$$

and realize that $K_\tau(\bar{x},\bar{x}')$ is a measurable and positive function on $D \times D$, whereas $K_{sf}(\bar{x},\bar{x}')$, which is also mea-

surable on $D \times D$, vanishes when $\Sigma_{sf}(\bar{x}') = 0$.

By introducing now the transformation T^*, generated by the kernel $K^*(\bar{x}, \bar{x}')$ and defined as

$$F^*(\bar{x}) = T^* f = \int_D K^*(\bar{x}, \bar{x}') f(\bar{x}') d_3\bar{x}', \tag{5}$$

where $F^*(\bar{x})$, T^*, and $K^*(\bar{x}, \bar{x}')$ stand for either $F_{sf}(\bar{x})$ or $F_\tau(\bar{x})$, T_{sf} or T_τ, $K_{sf}(\bar{x}, \bar{x}')$ or $K_\tau(\bar{x}, \bar{x}')$, respectively, and $f(\bar{x})$ is a function measurable on D, Eq. (2) can be formally cast into the operational form

$$\phi_0(\bar{x}) = T_{sf}\phi_0 + T_\tau Q = T_{sf}\phi_0 + \phi^Q, \tag{6}$$

ϕ^Q denoting the free term contributed by the distributed source Q.

The paper is organized along the following lines:

(i) In Sec. 2, by resorting to the finite double norm concept in a Lebesgue space $L_p(D)(p \geq 1)$, we study the general properties of the transport kernels $K_{sf}(\bar{x}, \bar{x}')$ and $K_\tau(\bar{x}, \bar{x}')$, Eq. (4), and of the corresponding transformations T_{sf} and T_τ, Eq. (5).

(ii) In Sec. 3, on the basis of the results of Sec. 2, taking any three-dimensional finite geometry and referring to the metrics of $L_p(D)$ with $p > 3$, we prove the convergence in the mean of the Neumann series solution associated with Eq. (2) and point out how the convergence depends on both the dimension and the nuclear properties of the system considered.

(iii) In Sec. 4 we list "practical" solutions to Eq. (2) which can be obtained once the transport kernel is approximated in the mean by a kernel of finite rank.

(iv) In Sec. 5 we consider Eq. (2) in the case where the source $Q(\bar{x})$ is an isotropic deltalike one, and briefly discuss how this case can be treated by means of a Fourier transform technique.

2. GENERAL PROPERTIES OF THE TRANSPORT KERNELS

A. Complete continuity of the transport kernels

We first notice that, in a system of the kind illustrated in the Introduction, the optical distance $\tau(\bar{x}, \bar{x}')$, Eq. (3), may be a discontinuous function with respect to both $\bar{x}$ and $\bar{x}'$. The continuity of $\tau(\bar{x}, \bar{x}')$ should be guaranteed by the additional assumptions:

(i) For any $\bar{x}$, every discontinuity surface S_i^* of the macroscopic cross section may be described by the polar equation

$$|\bar{x}_{s_i} - \bar{x}| = g_{i,\bar{x}}(\bar{\Omega}) \tag{7a}$$

where $\bar{\Omega} = \text{vers}(\bar{x}_{s_i} - \bar{x})$ and $\bar{x}_{s_i} \in S_i^*$, and

(ii) the function

$$g_{i,\bar{x}}(\bar{\Omega}) = g_{i,\bar{x}}(\theta, \varphi) \tag{7b}$$

is a continuous bounded function for every S_i^* and any fixed $\bar{x}$.

For instance, let us refer to the case where S_i^* is a plane, cylindrical, or conical surface, as may occur in the physical situation we are dealing with. The equation which represents a straight line on S_i^* passing through $\bar{x}$ is $\bar{\Omega} = \text{const}$, so that $g_{i,\bar{x}}(\bar{\Omega})$, Eqs. (7), is discontinuous. It is then seen that $\tau(\bar{x}, \bar{x}')$ is discontinuous for every pair $(\bar{x}, \bar{x}')$ belonging to the straight line, $\bar{\Omega} = \text{const}$, on S_i^*.

Returning now to the general problem of the continuity of $\tau(\bar{x}, \bar{x}')$, it can easily be inferred that the set, τ, of the points $\bar{x}$ at which $\tau(\bar{x}, \bar{x}')$, as a function of $\bar{x}'$ alone, becomes discontinuous, is a subset of D having zero measure. It follows from the symmetry of $\tau(\bar{x}, \bar{x}')$ that $e^{-\tau(\bar{x}, \bar{x}')}$ is continuous almost everywhere in $D \times D$.

As the discontinuity points of the bounded functions $\Sigma_{sf}(\bar{x})$ and $\Sigma(\bar{x})$ constitute a set of zero measure, we conclude by formulating the following theorem which is a generalization of a theorem quoted in Mikhlin[3] and guarantees the complete continuity of both the kernels $K_\tau(\bar{x}, \bar{x}')$ and $K_{sf}(\bar{x}, \bar{x}')$, Eq. (4), for the present physical situation:

Theorem: Let D be a closed and bounded domain of R_3, $0 \leq \alpha < 3$ a real number and $f(\bar{x}, \bar{x}')$ a measurable nonnegative bounded function, which is continuous almost everywhere in $D \times D$. Then any kernel of the type

$$t(\bar{x}, \bar{x}') = f(\bar{x}, \bar{x}')/4\pi|\bar{x} - \bar{x}'|^\alpha \tag{8}$$

is completely continuous in the Mikhlin sense, that is,

$$\lim_{\bar{x}_1 \to \bar{x}_2} \int_D |t(\bar{x}_1, \bar{x}') - t(\bar{x}_2, \bar{x}')| d_3\bar{x}' = 0 \tag{9}$$

uniformly for any pair $\bar{x}_1, \bar{x}_2 \in D$.

The proof of this theorem is given in Ref. 4.

B. The transport kernels, Eq. (4), as kernels of finite double norm

Hereafter we refer to a complete and separable Lebesgue space $L_p(D)$ with $p \geq 1$.

Let $t(\bar{x}, \bar{x}')$ be a measurable function on $D \times D$. Following Ref. 5 we say that $t(\bar{x}, \bar{x}')$ is of finite double norm $|||t|||$ on $D \times D$ if, for every pair of real numbers $p, q \geq 1$ such that

$$1/p + 1/q = 1, \tag{10}$$

there results

$$\begin{aligned} |||t||| &= \|t^{(q)}\|_p = [\int_D |t^{(q)}(\bar{x})|^p d_3\bar{x}]^{1/p} \\ &= \|\|t(\bar{x}, \bar{x}')\|_q\|_p \\ &= \{\int_D d_3\bar{x}[\int_D |t(\bar{x}, \bar{x}')|^q d_3\bar{x}']^{p/q}\}^{1/p} < \infty. \end{aligned} \tag{11}$$

Then $t(\bar{x}, \bar{x}')$ is also said to belong to the Banach space $N_p(D)$ with $p \geq 1$.

We pass now to show that both transport kernels, Eq. (4), are of finite double norm on $D \times D$ with $1 \leq q < \frac{3}{2}$ and $p > 3$. This is done by overestimating the kernels on the basis of the inequalities

$$\Sigma_{sf}(\bar{x}) \leq \Sigma_{sf}^{\max}, \qquad \Sigma(\bar{x}) \geq \Sigma_{\min} \geq 0, \tag{12}$$

which are in order for the present physical situation and hold for any $\bar{x} \in D$.

If Δ is the diameter of D defined as

$$\Delta = \sup_{\bar{x}, \bar{x}' \in D} |\bar{x} - \bar{x}'|, \tag{13}$$

we have, for the case $\Sigma_{\min} > 0$,

$$K_{sf}^{(q)}(\bar{x}) = \|K_{sf}(\bar{x},\bar{x}')\|_q \leq \Sigma_{sf}^{\max}/(4\pi)^{(q-1)/q} \times [\gamma(3-2q, q\,\Sigma_{\min}\Delta)/(q\,\Sigma_{\min})^{3-2q}]^{1/q} = h_{sf}^{(q)_1}, \quad (14)$$

which is recognized to converge for any real q such that

$$1 \leq q < \tfrac{3}{2}, \quad (14')$$

once we recall that, for $\mathrm{Re}\alpha > 0$, $\gamma(\alpha,u)$ denotes the incomplete gamma function.[6]

Introducing Eq. (14) into Eq. (11) yields

$$|||K_{sf}||| \leq h_{sf}^{(q)_1} \cdot V^{1/p} < \infty, \quad (15)$$

which expresses that, for $\Sigma_{\min} > 0$, $K_{sf}(\bar{x},\bar{x}')$ is of finite double norm on $D \times D$ for any real p such that

$$p > 3 \quad (15')$$

as follows by combining Eqs. (10) and (14').

The case $\Sigma_{\min} = 0$, which occurs when D includes voids, is treated in a similar way. Indeed, in the limit of $\Sigma_{\min} \to 0$ we get from Eqs. (14) and (15)

$$K_{sf}^{(q)}(\bar{x}) \leq \frac{\Sigma_{sf}^{\max}}{(4\pi)^{(q-1)/q}} \cdot \frac{\Delta^{(3-2q)/q}}{(3-2q)^{1/q}} = h_{sf}^{(q)_0} \quad (16a)$$

and

$$|||K_{sf}||| \leq h_{sf}^{(q)_0} \cdot V^{1/p} < \infty, \quad (16b)$$

respectively. Hence also for $\Sigma_{\min} = 0$ the kernel $K_{sf}(\bar{x}, \bar{x}')$ is of finite double norm on $D \times D$ for the same range of values of $q, p \geq 1$ quoted in Eqs. (14a) and (15a), respectively.

Inspection of Eqs. (14) and (16a) makes us aware of the important result that for both $\Sigma_{\min} \geq 0$, $K_{sf}^{(q)}(\bar{x}) = \|K_{sf}(\bar{x},\bar{x}')\|_q$ is actually bounded in D.

The same procedure can now be applied to the kernel $K_\tau(\bar{x},\bar{x}')$, which, like $K_{sf}(\bar{x},\bar{x}')$, belongs to $N_p(D)$ with $p > 3$: The norms $K_\tau^{(q)}(\bar{x})$ and $|||K_\tau|||$ are, in fact, recognized to admit bounds which coincide with those of the corresponding norms of $K_{sf}(\bar{x},\bar{x}')$ divided by $\Sigma_{sf}^{\max}$.

C. Properties of the transformations generated by the transport kernels

If in Eq. (5) $f(\bar{x})$ is a measurable function belonging to $L_p(D)$ with $p > 3$, by Hölder's inequality we deduce

$$|F^*(\bar{x})| = |T^*f| \leq \int_D |K^*(\bar{x},\bar{x}')f(\bar{x}')|\, d_3\bar{x}' \leq K^{*(q)}(\bar{x})\, \|f\|_p \leq h^{*(q)}\|f\|_p, \quad (17)$$

where $K^{*(q)}(\bar{x})$ stands for either $K_{sf}^{(q)}(\bar{x})$ or $K_\tau^{(q)}(\bar{x})$, and $h^{*(q)}$ for $h_{sf}^{(q)}$ or $h_\tau^{(q)}$.

Taking the norm of both sides of Eq. (17) yields

$$\|F^*\|_p = \|T^*f\|_p \leq |||K^*|||\, \|f\|_p \leq h^{*(q)} \cdot V^{1/p}\|f\|_p. \quad (18)$$

which expresses the well-known property that if a kernel belongs to $N_p(D)$, then the transformation generated by it is a linear integral transformation of $L_p(D)$ into $L_p(D)$. Such a transformation, which is bounded, is also compact and continuous. Keeping in mind that $K^{*(q)}(\bar{x})$ is bounded for any $\bar{x} \in D$, we may conclude that the transformations T_{sf} and T_τ generated by the transport kernels $K_{sf}(\bar{x},\bar{x}')$ and $K_\tau(\bar{x},\bar{x}')$, Eq. (4), are actually linear integral transformations of the Lebesgue space $L_p(D)$, with $p > 3$, into the space $B(D)$ of the functions bounded on D. Besides the space $B(D)$ we consider also the space $B_p(D)$ $(p \geq 1)$ of the functions which belong to $L_p(D)$ and which are almost everywhere bounded on D.

Now let $h(\bar{x})$ be a function belonging to $B_p(D)$ $(p \geq 1)$, that is, $|h(\bar{x})| < b$ = constant almost everywhere. Then we have

$$|H^*(\bar{x}_1) - H^*(\bar{x}_2)| \leq \int_D |K^*(\bar{x}_1,\bar{x}') - K^*(\bar{x}_2,\bar{x}')| \times |h(\bar{x}')|\, d_3\bar{x}' \leq b \int_D |K^*(\bar{x}_1,\bar{x}') - K^*(\bar{x}_2,\bar{x}')|\, d_3\bar{x}'. \quad (19)$$

As $K^*(\bar{x},\bar{x}')$ is completely continuous (see Sec. 2A), from Eq. (19) the uniform continuity of $H^*(\bar{x})$ on D follows. Thus T_{sf} and T_τ can also be regarded as linear integral transformations of $B_p(D)$ into $C_p(D)$, $C_p(D)$ being the space of the functions which are uniformly continuous on D. In $C_p(D)$ the norm is defined as in $L_p(D)$ $(p \geq 1)$.

3. THE NEUMANN SERIES SOLUTION

A. General properties of the solution of Eq. (2)

On the basis of Eqs. (17) and (19) we first observe that $T_\tau Q = \phi^Q$ [see Eq. (6)] belongs simultaneously to $C_p(D)$, $B_p(D)$, and $L_p(D)$ with $p \geq 1$.

Since the Fredholm alternative holds for any compact linear transformation of a Banach space,[5] in particular, for T_{sf} and $L_p(D)$ with $p > 3$ as in the present context, we can state that, if 1 is not an eigenvalue, a unique solution $\phi_0(\bar{x}) \in L_p(D)$ with $p > 3$ exists for Eq. (6).

On the other hand, still resorting to Eqs. (17) and (19), we realize that $T_{sf}\phi_0$ belongs to $B_p(D)$ so that $\phi_0 = T_{sf}\phi_0 + T_\tau Q \in B_p(D)$ and thence $T_{sf}\phi_0 \in C_p(D)$ with $p \geq 1$. We can thus conclude that $\phi_0 = T_{sf}\phi_0 + T_\tau Q$ belongs also to $C_p(D)$ with $p \geq 1$.

Therefore the solution $\phi_0(\bar{x})$ of Eq. (2), if 1 is not an eigenvalue, is unique and is represented by a uniformly continuous function on D belonging to all classes $L_p(D)$ with $p \geq 1$ even if $K_{sf}(\bar{x},\bar{x}')$ belongs to $N_p(D)$ with $p > 3$.

When $Q = \phi^Q = 0$ and 1 is an eigenvalue of the problem, the same considerations are in order: The solution $\phi_0(\bar{x})$ of the homogeneous form of Eq. (2) belongs to $C_p(D)$ and to $B_p(D) \subset L_p(D)$ with $p \geq 1$.

B. Convergence in the mean of the Neumann series solution

The Neumann series solution associated with Eq. (2) is formally

$$\tilde{\phi}_0(\bar{x}) = \sum_{n=0}^{\infty} (T_{sf})^n \phi^Q, \quad (20)$$

whose convergence in the mean is guaranteed, according to the Riesz–Fischer theorem, by the completeness of the Lebesgue space $L_p(D)$, once the Cauchy condition

$$\lim_{m,n\to\infty} \Big\| \sum_{i=m+1}^{n} (T_{sf})^i \phi^Q \Big\|_p = 0 \quad (21)$$

is satisfied.

By using Minkowski's inequality and the well-known result

$$\|(T_{sf})^n\| \leq \|T_{sf}\|^n \leq |||K_{sf}|||^n, \quad n = 1, 2, \ldots, \quad (22)$$

Eq. (21) can be rewritten as

$$\lim_{m,n\to\infty} \| \sum_{i=m+1}^{n} (T_{sf})^i \phi^Q \|_p \le \lim_{m,n\to\infty} \sum_{i=m+1}^{n} \| (T_{sf})^i \phi^Q \|_p \le \| \phi^Q \|_p \lim_{m,n\to\infty} \sum_{i=m+1}^{n} \| T_{sf} \|^i \le \| \phi^Q \|_p \lim_{m,n\to\infty} \sum_{i=m+1}^{n} |||K_{sf}|||^i, \tag{23}$$

where $p > 3$ as required in the present context.

From Eq. (23) we infer that the Cauchy condition, Eq. (21), is satisfied if

$$\| T_{sf} \| < 1 \tag{24a}$$

or, *a fortiori*, if

$$|||K_{sf}||| < 1, \tag{24b}$$

which thus represent the conditions sufficient for the Neumann series, Eq. (20), to converge in the mean (of index $p > 3$), to a function $\phi_0(\bar{x}) \in L_p(D)$, which is a solution of Eq. (2). In fact, by the continuity of the transformation T_{sf}, we get

$$T_{sf} \tilde{\phi}_0 = T_{sf} \sum_{n=0}^{\infty} (T_{sf})^n \phi^Q = \sum_{n=0}^{\infty} (T_{sf})^{n+1} \phi^Q = \tilde{\phi}_0 - \phi^Q. \tag{25}$$

That $\tilde{\phi}_0(\bar{x})$ is, apart from a set of zero measure, the unique solution of Eq. (2) follows from the Fredholm alternative since 1, as expressed by Eqs. (24), is not an eigenvalue of Eq. (2).

From Eqs. (17) and (22) we notice also that

$$| (T_{sf})^n \phi^Q | \le h_{sf}^{(q)} \| T_{sf} \|^{n-1} \| \phi^Q \|_p \le h_{sf}^{(q)} |||K_{sf}|||^{n-1} \| \phi^Q \|_p, \tag{26}$$

from which, using Eqs. (24), it is possible to demonstrate that the Neuman series, Eq. (20), is also absolutely and uniformly convergent and represents the unique and uniformly continuous solution of Eq. (2).

C. Explicit form for the sufficient conditions, Eqs. (24)

The condition $\| T_{sf} \| < 1$ cannot be easily handled as the overestimation of $\| T_{sf} \|$ implies the solution of a rather difficult extremal problem. Hence we confine ourselves to the more restrictive condition $|||K_{sf}||| < 1$, Eq. (24b), which, by Eqs. (15) and (16b), reduces to

$$\frac{\Sigma_{sf}^{\max}}{(4\pi)^{1/p}} \cdot \left(\frac{\gamma(3-2q, q\Sigma_{\min}\Delta)}{(q\Sigma_{\min})^{3-2q}} \right)^{1/q} \cdot V^{1/p} < 1, \tag{27a}$$

when $\Sigma_{\min} > 0$ and

$$\frac{\Sigma_{sf}^{\max}}{(4\pi)^{1/p}} \cdot \left(\frac{\Delta^{3-2q}}{3-2q} \right)^{1/q} \cdot V^{1/p} < 1, \tag{27b}$$

when $\Sigma_{\min} = 0$, respectively.

In the limit of $u = q\Sigma_{\min}\Delta \ll 1$, that is, for very small systems, since $\gamma(\alpha, u) \simeq \alpha^{-1} \cdot u^{\alpha}$, Eq. (27a) reduces to Eq. (27b).

On the contrary, when $u = q\Sigma_{\min}\Delta \gg 1$, that is, for very large systems, in Eq. (27a), $\gamma(\alpha, u)$ can be replaced by the gamma function $\Gamma(\alpha)$.[6]

Returning to Eqs. (27), we now take $p = \infty$, hence $q = 1$. This is meaningful as we have found that a unique solution of Eq. (2) exists which is bounded on the closed finite domain D.

The sufficient condition, Eq. (24b), then reads as

$$\frac{\Sigma_{sf}^{\max}}{\Sigma_{\min}} \gamma(1, \Sigma_{\min}\Delta) = \frac{\Sigma_{sf}^{\max}}{\Sigma_{\min}} (1 - e^{-\Sigma_{\min}\Delta}) < 1, \tag{28a}$$

when $\Sigma_{\min} > 0$ and

$$\Sigma_{sf}^{\max} \Delta < 1, \tag{28b}$$

when $\Sigma_{\min} = 0$. Both equations (28) coincide in the limit of $\Sigma_{\min}\Delta \ll 1$.

The physical interpretation to be attached to the explicit conditions above derived for the convergence of the Neumann series, Eq. (20), follows immediately from a comparison, for any fixed Δ, of the effects of the neutron absorption and escape with the neutron production by scattering and fission.

4. PRACTICAL SOLUTIONS FOR EQ. (2)

A. General remarks

Since the explicit evaluation of the general term of the Neumann series, Eq. (20), is a very arduous task, we pass now, as usual in many problems of mathematical physics, to consider the problem of constructing a "practical" solution for Eq. (2). We shall accomplish this task by extending to the present three-dimensional systems the procedure proposed in Ref. 7 for the case of a mono-dimensional infinite slab of finite thickness. This procedure consists of approximating the kernel of Eq. (2) in the mean by a kernel of finite rank.

For the sake of simplicity, we shall first refer to convex finite bodies made of a homogeneous material, that is, in Eqs. (1), $\Sigma(\bar{x}')$ and $\Sigma_{sf}(\bar{x}')$ are now independent of position. Equation (2) then becomes

$$\phi_0(\bar{x}) = \Sigma_{sf} \int_D K(\bar{x}, \bar{x}') \phi_0(\bar{x}') d_3\bar{x}' + \phi^Q(\bar{x}), \tag{29}$$

whose Kernel

$$K(\bar{x}, \bar{x}') = e^{-\Sigma|\bar{x}-\bar{x}'|}/4\pi|\bar{x} - \bar{x}'|^2 \tag{30}$$

is easily recognized as belonging to $N_p(D)$ with $p > 3$, like the corresponding kernel of Eq. (2). In particular, we shall exploit in the sequel the circumstance that, as a function of $\bar{x}'$ alone, the kernel $K(\bar{x}, \bar{x}')$, Eq. (30), is of class $L_1(D)$, as follows from Eq. (14).

B. The approximation of the kernel, Eq. (30)

Let $x_l' \in I_l(a_l, b_l)$ $(l = 1, 2, 3)$ be the coordinate of the general point $\bar{x}' \in D$ with respect to an arbitrary three-dimensional reference system $I_l(a_l, b_l)$ denoting a closed finite interval.

As $K(\bar{x}, \bar{x}')$ is of class $L_1(D)$ it follows from Fubini's theorem that, for any $\bar{x} \in D$, $K(\bar{x}, \bar{x}')$ is summable over I_l, namely

$$\chi(\bar{x}, x_i', x_j') = \int_D |K(\bar{x}, \bar{x}')| dx_l' < \infty, \quad i \ne j \ne l \; i,j,l = 1, 2, 3) \tag{31}$$

for almost every $x_i' \in I_i$ and $x_j' \in I_j$.

Let us now take the infinite countable sequence

$\{\psi^l_{n_l}(x'_l)\}$ $(l = 1, 2, 3, n_l = 1, 2, \ldots)$ of polynomials of a degree coincident with their index. This sequence is then complete in I_l, and we suppose that it is also orthonormalized with respect to the weight function $w_l(x'_l)$, that is,

$$\int_{I_l} w_l(x'_l)\psi^l_{n_l}(x'_l)\psi^l_{m_l}(x'_l)\,dx'_l = \delta_{n_l m_l}, \tag{32}$$

where $\delta_{n_l m_l}$ is the Kronecker index. For later reference we recall that the linear manifold determined by $\{\psi^l_{n_l}(x'_l)\}$, that is, the set of all finite linear combinations $\sum_l \alpha_{n_l}\psi^l_{n_l}(x'_l)$, is everywhere dense in $L_1(I_l)$. By choosing the α_{n_l} as rational complex numbers, we can recognize that $L_1(I_l)$ is separable.

We then form the infinite countable sequence

$$\{G_{n_1n_2n_3}(\bar{x}')\} = \left\{\prod_{l=1}^{3}\psi^l_{n_l}(x'_l)\right\}, \tag{33}$$

which, like the sequence $\{\psi^l_{n_l}(x'_l)\}$, is complete and can determine a linear manifold, everywhere dense in $L_1(D)$. The space $L_1(D)$ is thus separable as already stipulated for the space $L_1(I_l)$.

As far as the orthonormality properties of the functions $G_{n_1n_2n_3}(\bar{x}')$ are concerned, we realize that, if the general weight function $w_l(x'_l)$ is chosen so that $d_3\bar{x}' = \prod_{l=1}^{3} w'_l(x'_l)dx'_l$, we obtain

$$\int_D G_{n_1n_2n_3}(\bar{x}')G_{m_1m_2m_3}(\bar{x}')d_3\bar{x}' = \delta_{n_1m_1}\delta_{n_2m_2}\delta_{n_3m_3}. \tag{34}$$

In Table I we list the values of the three weight functions $w_1(x_1), w_2(x_2), w_3(x_3)$ for the most common systems of coordinates. We list also the corresponding variation range of the considered coordinate defining the closed finite domain D.

TABLE I.

Coordinates	$w_1(x_1)$	$w_2(x_2)$	$w_3(x_3)$	I_1	I_2	I_3
Cartesian (x_1, x_2, x_3)	1	1	1	$(-\alpha_1, \alpha_1)$	$(-\alpha_2, \alpha_2)$	$(-\alpha_3, \alpha_3)$
cylindrical $(x_1 = \rho; x_2 = \chi; x_3 = z)$	ρ	1	1	$(0, R)$	$(0, 2\pi)$	$(-H, H)$
spherical $(x_1 = r; x_2 = \theta; x_3 = \psi)$	r^2	$\sin\theta$	1	$(0, R)$	$(0, \pi)$	$(0, 2\pi)$

With all this information at hand let us now expand the kernel $K(\bar{x}, \bar{x}')$, Eq. (30), regarded as a function of $\bar{x}'$ alone, in terms of the functions $G_{n_1n_2n_3}(\bar{x}')$, Eq. (33), by writing

$$K(\bar{x}, \bar{x}') = \sum_{n_1,n_2,n_3=0}^{\infty} F_{n_1n_2n_3}(\bar{x})G_{n_1n_2n_3}(\bar{x}'), \tag{35}$$

where

$$F_{n_1n_2n_3}(\bar{x}) = \int_D K(\bar{x}, \bar{x}')G_{n_1n_2n_3}(\bar{x}')d_3\bar{x}' \tag{36}$$

is a sort of Fourier coefficient of $K(\bar{x}, \bar{x}')$ with respect to the assigned sequence, Eq. (33).

For any triplet $N_1, N_2, N_3 > 0$ we now set

$$K(\bar{x}, \bar{x}') = L_{N_1N_2N_3}(\bar{x}, \bar{x}') + M_{N_1N_2N_3}(\bar{x}, \bar{x}') \tag{37}$$

with

$$L_{N_1N_2N_3}(\bar{x}, \bar{x}') = \sum_{n_1=0}^{N_1}\sum_{n_2=0}^{N_2}\sum_{n_3=0}^{N_3} F_{n_1n_2n_3}(\bar{x})G_{n_1n_2n_3}(\bar{x}'). \tag{38}$$

As the infinite countable sequence $G_{n_1n_2n_3}(\bar{x}')$ is complete in $L_1(D)$, we have

$$\lim_{N_1,N_2,N_3\to\infty} \|K(\bar{x}, \bar{x}') - L_{N_1N_2N_3}(\bar{x}, \bar{x}')\|_1 = \lim_{N_1,N_2,N_3\to\infty} \|M_{N_1N_2N_3}(\bar{x}, \bar{x}')\|_1 = 0 \tag{39}$$

in agreement with the separability of $L_1(D)$.

Equation (39) expresses that, for any $\bar{x} \in D$, the triple series on the rhs of Eq. (35) is convergent in the mean (of index $p = 1$) to the kernel, Eq. (30). We thus recognize that, whereas $L_{N_1N_2N_3}(\bar{x}, \bar{x}')$, Eq. (38), is a kernel of finite rank, $M_{N_1N_2N_3}(\bar{x}, \bar{x}')$ is a kernel whose norm, according to Eq. (39), can be made as small as desired. Hence the approximation of setting, for any $\bar{x} \in D$,

$$K(\bar{x}, \bar{x}') \simeq L_{N_1N_2N_3}(\bar{x}, \bar{x}'), \tag{40}$$

is just the approximation of kernel $K(\bar{x}, \bar{x}')$, Eq. (30), sought.

C. Practical solution of Eq. (29)

First we introduce Eq. (35) for $K(\bar{x}, \bar{x}')$ into Eq. (29). Then by the convergence in the mean of the triple series on the rhs of Eq. (35) and by the boundedness of $\phi_0(\bar{x})$ we may exchange the order of integration and summation in the integral term of Eq. (29) (see Appendix), so that we obtain

$$\phi_0(\bar{x}) = \Sigma_{sf}\sum_{n_1,n_2,n_3=0}^{\infty} \xi_{n_1n_2n_3}F_{n_1n_2n_3}(\bar{x}) + \phi^q(\bar{x}), \tag{41}$$

where the coefficients

$$\xi_{n_1n_2n_3} = \int_D G_{n_1n_2n_3}(\bar{x}')\phi_0(\bar{x}')d_3\bar{x}' \tag{42}$$

are finite as $G_{n_1n_2n_3}(\bar{x}')$ and $\phi_0(\bar{x}')$ are bounded on D.

When the general n_l is restricted to some finite integer $N_l[0 \le n_l \le N_l\ (l = 1, 2, 3)]$, Eq. (41) represents the sought practical solution of Eq. (29) in terms of the known functions $F_{n_1n_2n_3}(\bar{x})$, Eq. (36), and of the free term $\phi^q(\bar{x})$, once the coefficients $\xi_{n_1n_2n_3}$ are determined by resorting to the orthonormality properties, Eq. (34), of the sequence $\{G_{n_1n_2n_3}(\bar{x})\}$. In fact, multiplying throughout Eq. (41) by $G_{m_1m_2m_3}(\bar{x})$ and integrating over D, we are left with the infinite algebraic system

$$\xi_{m_1m_2m_3} = \Sigma_{sf}\sum_{n_1,n_2,n_3=0}^{\infty} A^{m_1m_2m_3}_{n_1n_2n_3}\xi_{n_1n_2n_3} + B_{m_1m_2m_3}, \tag{43}$$

where both the integrals

$$A^{m_1m_2m_3}_{n_1n_2n_3} = \int_D G_{m_1m_2m_3}(\bar{x})F_{n_1n_2n_3}(\bar{x})d_3\bar{x} \tag{44a}$$

and

$$B_{m_1m_2m_3} = \int_D G_{m_1m_2m_3}(\bar{x})\phi^q(\bar{x})d_3\bar{x} \tag{44b}$$

are easily recognized to be finite.

When $Q(\bar{x}) = \phi^q(\bar{x}) = 0$, we have $B_{m_1m_2m_3} = 0$ so that Eqs. (41) and (43) constitute an eigenvalue problem.

The polynomials $\psi^l_{n_l}(x_l)$ to be used in Eq. (33) are still to be chosen. We shall confine our attention to the Legendre polynomials whose argument will be specified in the next paragraph for three typical convex finite geometries.

D. Examples

The domain D is taken to be successively a parallelepiped of dimension $2\alpha_l$ along the coordinate axis $Ox_l (l = 1, 2, 3)$, a cylinder of radius R and of height $2H$, and a sphere of radius R (compare Table I). The origin of the corresponding coordinate system coincides with the center of domain D. With a distributed source $Q(\bar{x})$ having the same symmetry as the coordinate system being considered, the results of the application of the theory illustrated in the two preceding paragraphs are the following:

(i) *parallelepiped*

$$\phi_0(\bar{x}) = \phi_0(x_1, x_2, x_3),$$

$$K(\bar{x}, \bar{x}') = \frac{\exp\left\{-\Sigma\left[\sum_{l=1}^{3}(x_l - x_l')^2\right]^{1/2}\right\}}{4\pi \sum_{l=1}^{3}(x_l - x_l')^2}, \tag{45a}$$

$$G_{n_1n_2n_3}(\bar{x}') = \prod_{l=1}^{3}\left(\frac{2n_l + 1}{2\alpha_l}\right)^{1/2} \cdot P_{n_l}\left(\frac{x_l'}{\alpha_l}\right),$$

$$A^{m_1m_2m_3}_{n_1n_2n_3} = 0 \quad \text{for } m_l + n_l \text{ odd},$$

$$B_{m_1m_2m_3} = 0 \quad \text{for } m_l \text{ odd} \quad (l = 1, 2, 3).$$

(ii) *cylinder*

$$\phi_0(\bar{x}) = \phi_0(\rho, \chi, z) \to \phi_0(\rho, z),$$

$$K(\bar{x}, \bar{x}') \to K(\rho, z; \rho', z') = \int_0^{2\pi} \times \frac{\exp\{-\Sigma[\rho^2 + \rho'^2 - 2\rho\rho'\cos(\chi - \chi') + (z - z')^2]^{1/2}\}}{4\pi[\rho^2 + \rho'^2 - 2\rho\rho'\cos(\chi - \chi') + (z - z')^2]} d\chi',$$

$$G_{n_1n_2n_3}(\bar{x}') \to G_{n_\rho n_z}(\rho', z') = \frac{[2(2n_\rho + 1)]^{1/2}}{R} \cdot P_{n_\rho}\left(1 - 2\frac{\rho'^2}{R^2}\right) \times \left(\frac{2n_z + 1}{2H}\right)^{1/2} \cdot P_{n_z}\left(\frac{z'}{H}\right), \tag{45b}$$

$$A^{m_\rho m_z}_{n_\rho n_z} = 0 \quad \text{for } m_z + n_z \text{ odd},$$

$$B_{n_\rho n_z} = 0 \quad \text{for } n_z \text{ odd}.$$

(iii) *sphere*

$$\phi_0(\bar{x}) = \phi_0(r, \theta, \varphi) \to r\phi_0(r),$$

$$K(\bar{x}, \bar{x}') \to K(r, r') = \tfrac{1}{2} E_1(\Sigma|r - r'|),$$

$$G_{n_1n_2n_3}(\bar{x}') \to G_{n_r}(r') = \left(\frac{2n_r + 1}{2R}\right)^{1/2} \cdot P_{n_r}\left(\frac{r'}{R}\right). \tag{45c}$$

Extension of the results of this section to the general case represented by Eq. (2) is immediate once the kernel $K_{sf}(\bar{x}, \bar{x}')$ of Eq. (2) is recalled to possess all the properties which have been already invoked for the kernel $K(\bar{x}, \bar{x}')$ of Eq. (29) in the limiting case of constant cross sections.

The solution of Eq. (2) is still of the form of Eq. (41), provided we replace $\Sigma_{sf} F_{n_1n_2n_3}(\bar{x})$ by

$$F^*_{n_1n_2n_3}(\bar{x}) = \int_D \Sigma_{sf}(\bar{x}') \frac{e^{-\tau(\bar{x}, \bar{x}')}}{4\pi|\bar{x} - \bar{x}'|^2} G_{n_1n_2n_3}(\bar{x}') d_3\bar{x}', \tag{45d}$$

which takes into account the inhomogeneity of cross sections. In Eq. (45d) $G_{n_1n_2n_3}(\bar{x})$ is still an element of the infinite countable sequence, Eq. (33).

In turn the coefficients $\xi_{n_1n_2n_3}$ still satisfy the system (43), in which $\Sigma_{sf} A^{m_1m_2m_3}_{n_1n_2n_3}$ is now replaced by

$$A^{*m_1m_2m_3}_{n_1n_2n_3} = \int_D G_{m_1m_2m_3}(\bar{x}) F^*_{n_1n_2n_3}(\bar{x}) d_3\bar{x}$$

with $F^*_{n_1n_2n_3}(\bar{x})$ given by Eq. (45d).

Of course the known terms $B_{m_1m_2m_3}$, Eq. (44b), of system (43) must be evaluated by exploiting the appropriate definition, Eq. (6), for the free term $\phi^q(\bar{x})$ of Eq. (2).

5. THE CASE OF AN ISOTROPIC DELTALIKE SOURCE IN A HOMOGENEOUS SYSTEM

A. General remarks

When the neutron source $Q(\bar{x})$ is no longer distributed but is an isotropic deltalike one, namely

$$Q(\bar{x}) = Q\delta(\bar{x}), \tag{46a}$$

the free term of Eq. (29) becomes

$$\phi^q(\bar{x}) = Qe^{-\Sigma|\bar{x}|}/4\pi|\bar{x}|^2 = Q\psi(\bar{x}) \tag{46b}$$

as follows from its general definition, Eqs. (5) and (6).

In this case, whereas the kernel $K(\bar{x}, \bar{x}')$ of Eq. (29) still belongs to $N_p(D)$ with $p > 3$, the free term $\phi^q(\bar{x})$, Eq. (46b), belongs instead to $L_q(D)$ $(1 \le q < 3/2)$, which is complementary to $L_p(D)$ $(p > 3)$. Indeed, proceeding as was done in the case of Eq. (14), we find that

$$\|\phi^q\|_q = \frac{Q}{(4\pi)^{(q-1)/q}} \cdot \left(\frac{\gamma(3 - 2q, q\Sigma\Delta)}{(q\Sigma)^{3-2q}}\right)^{1/q}, \tag{47}$$

which in fact converges for $3 - 2q > 0$.

Furthermore, we realize that

(i) the application of the transformation T with kernel $K(\bar{x}, \bar{x}') \in N_p(D)$ to the function $\phi^q(\bar{x}) \in L_q(D)$ no longer guarantees, in general, that the resulting function will still be of class $L_q(D)$;

(ii) the solution $\phi_0(\bar{x})$ of Eq. (29) cannot be any longer proved in general to be continuous and bounded on D.

This two-fold inconsistency, which as a consequence of the choice of the source, Eq. (46a), emerges in the theory so far developed, can be overcome, as shown hereunder, once Eq. (29) is regularized through a technique based on the Fourier transform.

B. Fourier transform of Eq. (29)

By introducing the characteristic function $p_V(\bar{x})$ of volume V of domain D, Eq. (29) can be rewritten as

$$\phi_0(\bar{x}) = \Sigma_{sf} \int_{R_3} \psi(\bar{x} - \bar{x}')p_V(\bar{x}')\phi_0(\bar{x}')d_3\bar{x}' + Q\psi(\bar{x}), \quad (48)$$

where $\psi(\bar{x})$ is defined by Eq. (46b).

Taking a three-dimensional Fourier transform of both sides of Eq. (48) and denoting by $\tilde{h}(\bar{B})$ (where $\bar{B}$ is the vector associated to the transformation) the Fourier transform of $h(\bar{x})$, we obtain as a consequence of a two-fold application of the convolution theorem

$$\tilde{\phi}_0(\bar{B}) = \Sigma_{sf}\tilde{\psi}(\bar{B}) \frac{1}{(2\pi)^3} \int_{R_{F3}} \tilde{p}_V(\bar{B} - \bar{B}')\tilde{\phi}_0(\bar{B}')d_3\bar{B}' + Q\tilde{\psi}(\bar{B}), \quad (49)$$

which is a linear integral equation in $R_{F3} \equiv R_3$ for the Fourier transform $\tilde{\phi}_0(\bar{B})$ of the unknown $\phi_0(\bar{x})$ and is of the same form as Eq. (2.12) of Ref. 1.

That Eq. (49) is the sought regularized form of the original Equation (29) in the case of the source, Eq. (46a), can be seen as follows.

We first notice that

$$\tilde{\psi}(\bar{B}) = \frac{\tan^{-1}B/\Sigma}{B} < 1/\Sigma. \quad (50)$$

where $B = |\bar{B}|$, is a continuous bounded function for $0 \le B \le \infty$ and is of class $L_p(R_{F3})$ with $p > 3$. In fact its norm

$$\|\tilde{\psi}\|_p = [\int_{R_{F3}} |\tilde{\psi}(\bar{B})|^p d_3\bar{B}]^{1/p} = \left(4\pi\Sigma^{3-p}\int_0^\infty \frac{(\tan^{-1}r)^p}{r^{p-2}}dr\right)^{1/p} \quad (51)$$

clearly converges for $p > 3$.

On the other hand for the double norm of the kernel

$$\tilde{K}(\bar{B},\bar{B}') = (2\pi)^{-3}\tilde{\psi}(\bar{B})\tilde{p}_V(\bar{B} - \bar{B}') \quad (52)$$

of Eq. (49) we find, according to the definition of Eq. (11), that

$$|||\tilde{K}||| = (2\pi)^{-3} \cdot \|\tilde{\psi}\|_p \cdot [\int_{R_{F3}} |\tilde{p}_V(\bar{B}'')|^q d_3\bar{B}'']^{1/q}. \quad (53)$$

When the bracketed integral turns out to converge for $a_g \le q < \frac{3}{2}$, where $a_g \ge 1$ is a real number depending on geometry, we deduce, according to Eq. (10), that $\tilde{K}(\bar{B},\bar{B}') \in N_p(R_{F3})$ with $a_g/a_g - 1 \ge p > 3$. This occurs, for instance, in the parallelepiped case with $a_g = 1$. If the bracketed integral on the rhs of Eq. (53) do not converge for $a_g \le q < \frac{3}{2}$, the regularization could be attained by exploiting the symmetry of both geometry and source through a reduction of the number of independent variables to be considered.

Once $\tilde{K}(\bar{B},\bar{B}')$ is verified to belong to $N_p(R_{F3})$ with $p > 3$, the discussion of Eq. (49) is amenable to that of the kind developed for Eq. (2): among other things, in the case of Eq. (49), the closed finite domain D is replaced by $R_{F3} \equiv R_3$.

We recall that Eq. (49) has already been investigated by a Fourier transform technique, more or less similar to the one here illustrated, in Refs. 8–12 for the parallelepiped, cylinder of finite height, sphere, mono-dimensional slab of finite thickness and cylinder of infinite height, respectively. It is interesting to remark that for the first three of the geometries mentioned above the results, obtained by transforming back the practical solution of Eq. (49), once the Kernel $\tilde{K}(\bar{B},\bar{B}')$, Eq. (52), is expressed in $R_{F3} \times R_{F3}$ as a bilinear series in terms of Bessel functions, exactly coincide with those quoted in Eqs. (45a)–(45c).

APPENDIX

The change of the order of integration and summation in the integral term of Eq. (29) can be justified as follows.

By the boundedness of $\phi_0(\bar{x})$ we first have

$$\begin{aligned} &|\int_D [K(\bar{x},\bar{x}') - L_{N_1N_2N_3}(\bar{x},\bar{x}')]\phi_0(\bar{x}')d_3\bar{x}'| \\ &\quad \le \int_D |K(\bar{x},\bar{x}') - L_{N_1N_2N_3}(\bar{x},\bar{x}')|\,|\phi_0(\bar{x}')|d_3\bar{x}' \\ &\quad \le M \cdot \|K(\bar{x},\bar{x}') - L_{N_1N_2N_3}(\bar{x},\bar{x}')\|_1. \end{aligned} \quad (A1)$$

Then, on the basis of Eq. (39),

$$\lim_{N_1,N_2,N_3\to\infty} |\int_D [K(\bar{x},\bar{x}') - L_{N_1N_2N_3}(\bar{x},\bar{x}')]\phi_0(\bar{x}')d_3\bar{x}'| = 0, \quad (A2)$$

so that

$$\begin{aligned} \int_D \lim_{N_1,N_2,N_3\to\infty} L_{N_1N_2N_3}(\bar{x},\bar{x}')\phi_0(\bar{x}')d_3\bar{x}' &= \int_D K(\bar{x},\bar{x}')\phi_0(\bar{x}')d_3\bar{x}' \\ &= \lim_{N_1,N_2,N_3\to\infty} \int_D L_{N_1N_2N_3}(\bar{x},\bar{x}')\phi_0(\bar{x}')d_3\bar{x}', \end{aligned} \quad (A3)$$

which precisely expresses the Lebesgue theorem for term by term integration in the present case.

From Eq. (A3) one gets Eq. (41), once the position of Eq. (42) is accounted for.

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*Work supported by CNR, National Research Council, Rome, Italy.
†Work performed during the preparation of the thesis for the degree of "Dottore in Ingegneria Nucleare."

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Current algebras of free systems at finite temperature

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(Received 22 May 1972)

This paper is a study of the representations of the current algebra for an infinite, free, Bose or Fermi system at finite temperature. The state of the algebra is calculated for a finite system by use of the grand canonical formalism of statistical physics, and the thermodynamic limit is used to get the representation of the infinite case. An expression of the states is given in terms of determinants of one particle operators. In a second part, the usual formulas for the occupation density, the condensation temperature for bosons, etc., are recovered. It is also found that the canonical and grand canonical formalisms are equivalent when used to study Fermi systems in the thermodynamic limit, but not so for the Bose systems. It is postulated that this has something to do with the phase transition of Bose systems. Finally, the problem of the Hamiltonian is discussed in some details. The states calculated previously are used to test a method for calculating expectation values of the Hamiltonian, given the states of the algebra; it yields the correct value for the case of the free system at finite temperature.

INTRODUCTION

It is evident from a brief examination of the literature on axiomatic physics that a strong emphasis has been given to the algebraic aspect of field theories. At the same time, it has also been suggested that the ordinary canonical formalism used to describe such theories might be replaced by other coordinates, and especially the so-called Current fields.[1-6] It is the purpose of this work to describe a simple physical system, a free gas at finite temperature, in terms of such fields, and in the context of the theory of representations of a C^*-algebra.

The work is divided as follows. The general properties of C^*-algebras are reviewed, and the possible forms of the Hamiltonian are discussed. In the second section, symmetric functions are introduced, and expressed in terms of traces of Hermitian operators; then, general formulas are demonstrated that will be of use in subsequent chapters. In the third part, the state of the exponentiated group of the current algebra is computed for a free gas at finite temperature in a finite box Section IV deals with the thermodynamic limit of the state by use of the grand canonical formalism, and the questions of convergence and Bose condensation are discussed. A method for computing the Hamiltonian is also described and applied to the free system.

I. ALGEBRA AND FIELD THEORIES

This section will deal mostly with two topics: the algebraic aspect of field theories, and the problem of the Hamiltonian in current algebra.

A. C^*-algebras

All the proofs of the properties of C^*-algebras that follow can be found in Dixmier.[7] Let $\mathfrak{A}$ denote an algebra and * an involution over the field of complex numbers, i.e. for $A \in \mathfrak{A}$, $A^* \in \mathfrak{A}$, with the properties

$$(A^*)^* = A,$$
$$(A + aB)^* = A^* + \bar{a}B^*,$$
$$(AB^*) = B^*A^*.$$

A B^*-algebra is an algebra $\mathfrak{A}$ over the field C of complex numbers with norm $\|A\|$ and involution * such that

$$\|A^*\| = \|A\|,$$
$$\|A_1A_2\| \leq \|A_1\| \, \|A_2\|,$$
$$\|A^*A\| = \|A\|^2.$$

C^*-algebra: If we have a Hilbert space $\mathfrak{H}$ and $\mathfrak{B}(\mathfrak{H})$ = the set of bounded linear operators on $\mathfrak{H}$. If $A \in \mathfrak{B}(\mathfrak{H})$, and A^* is the usual adjoint operator, $\|A\|$ is defined as

$$\|A\| = \sup\|A\phi\|, \qquad \|\phi\| \leq 1.$$

A subalgebra $\mathfrak{A}$ of $\mathfrak{B}(\mathfrak{H})$ which is self-adjoint, i.e., $A \in \mathfrak{A} \Rightarrow A^* \in \mathfrak{A}$, and norm-closed, is a C^*-algebra. Any C^*-algebra is a B^*-algebra, and conversely, every B^*-algebra is isomorphic to a C^*-algebra on some $\mathfrak{H}$. In all the statements that will follow, we will assume that the algebras have an identity I.

A representation of a B^* algebra on a Hilbert space is a map Π: $\mathfrak{A} \to$ linear bounded or unbounded operators on $\mathfrak{H}$. This map must preserve the algebraic structure, i.e., if A and $B \in \mathfrak{A}$

$$\Pi(A)\Pi(B) = \Pi(AB),$$
$$\Pi(A^*) = \Pi(A)^*.$$

A representation is said to be cyclic if $\exists\, \Omega \in \mathfrak{H} \to \mathfrak{A}\,\Omega \subsetneq \mathfrak{H}$. The vector Ω is said to be a cyclic vector.

The states ρ on $\mathfrak{A}$ are continuous linear functionals on $\mathfrak{A}$, positive and normalized to 1; if $A \in \mathfrak{A}$, A is said to be positive if

$$A = B^*B \text{ for some } B \in \mathfrak{A}$$

and we write $A > 0$.

A state $\rho(A)$ is positive if for $A > 0$, $\rho(A) > 0$. The state is normalized to unity if $\rho(I) = 1$.

The Gel'fand–Segal construction: There is an important relation between states and representations of a B^*-algebra. If there exists a cyclic representation Π of the algebra $\mathfrak{A}$ with a cyclic vector Ω, then $\rho(A) = (\Omega, \Pi(A)\Omega)$ defines a state on the algebra. The converse also holds, namely that a state on the algebra defines a cyclic representation up to a unitary equivalence. This theorem is the basis upon which this work will rest; we will compute a state for the current algebra, and because of the Gel'fand–Segal construction, this state will be sufficient to describe the physical system completely.

Equivalent representations: Two representations Π_1 and Π_2 in $\mathfrak{H}_1$ and $\mathfrak{H}_2$, respectively, are said to be equivalent if there exists an isometry V of $\mathfrak{H}_1$ onto $\mathfrak{H}_2$ such that

$$\Pi_2(A) = V\Pi_1(A)V^{-1}.$$

It is shown that two representations Π_1 and Π_2 in $\mathfrak{H}_1$ and $\mathfrak{H}_2$ respectively are equivalent if and only if there exists a cyclic $\Omega_2 \in \mathfrak{H}_2$ such that

$$(\Omega_1, \Pi_1(\mathfrak{A})\Omega_1) = (\Omega_2, \Pi_2(\mathfrak{A})\Omega_2).$$

Irreducible representations: A representation Π of a B^*-algebra $\mathfrak{A}$ is said to be irreducible if given $C \in \mathfrak{B}(\mathfrak{H})$ and $[C, \Pi(A)] = 0$ for all $A \in \mathfrak{A}$, then $C = aI$. In terms of states, this condition for irreducibility is equivalent to having a pure state. If $\rho = \lambda\rho_1 + (1-\lambda)\rho_2$ with ρ_1 and ρ_2 states, and $0 \leq \lambda \leq 1$, ρ is pure if and only if the only possible such decomposition is $\rho = \rho_1 = \rho_2$.

B. Canonical and current fields

We see that the properties of reducibility and equivalence of representations can be discussed entirely in terms of states and that these states define a cyclic representation up to a unitary equivalence. We will now give specific examples of C^*-algebras used to describe physical systems.

The C^*-algebra usually encountered in physics is the algebra of canonical fields. It can be characterized as the algebra of all polynomials in the quantities $\phi(x)$ and $\Pi(y)$, subject to the conditions of commutation or anticommutation

$$[\phi(x), \Pi(y)]_\pm = i\delta(x-y)$$

with the + (−) sign referring to fermions (bosons). There is, of course, one very well-known representation for such an algebra, the Fock representation. The Hilbert space for the representation is denoted $\oplus_N \mathfrak{H}_N$, where $\mathfrak{H}_N$ is the N-particle subspace and is the set of square-integrable functions in N variables that obey symmetric or antisymmetric statistics, with the constraint that, for all $\psi \in \mathfrak{H}$,

$$\sum_{N=0}^{\infty} (\psi_N, \psi_N) = (\psi, \psi) < \infty$$

and (ψ_N, ψ_N) is the usual L^2 inner product. We will give the representation of the smeared fields

$$\phi(f) = \int f(x)\phi(x)dx, \quad \Pi(g) = \int \Pi(x)g(x)dx,$$

and f and g are either Schwartz functions or functions of compact support in the box.

Define the auxiliary fields

$$a(f) = [\phi(f) + i(\Pi(f)]/\sqrt{2}, \quad a^*(f) = [\phi(f) - i\Pi(f)]/\sqrt{2}.$$

On the N-particle sector, for Bose statistics, the Fock representation for the a's and a^*'s is

$$(a(f)\psi_N)(x_1 \ldots x_N) = \sqrt{N+1}\int \psi_{N+1}(x_1 x_2 \ldots x_N, x)f(x)dx,$$

$$(a^*(f)\psi_N)(x_1 \ldots x_N) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \overline{f(x_i)}\psi_{N-1}(x_1 \hat{x}_1 \ldots x_N),$$

where $\hat{x}_i$ means that the coordinate x_i is to be omitted.

For the anticommutation relations, we get

$$(a(f)\psi_N)(x_1 \ldots x_N) = \sqrt{N+1}\int \psi_{N+1}(x_1 \ldots x_N, x)f(x)dx,$$

$$(a^*(f)\psi_N)(x_1 \ldots x_N) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i+1}\overline{f}(x_i)\psi_{N-1}(x_1 \ldots \hat{x}_i \ldots x_N).$$

It is easy to check that these fields satisfy the expected commutation or anticommutation relations,

$$[a(f), a^*(g)]_\pm = \int f(x)g(x)dx.$$

It is now appropriate to make some comments on the representations of the canonical fields, since it will indicate some of the reasons for the procedure used later.

First, it is well known that although the Fock representation is bounded for Fermi fields, it is not so for the Bose fields.

Mathematical properties of unbounded representations of canonical fields have been investigated,[8] but the usual procedure is to consider representations of the group of exponentiated operators, the Weyl group. Once this group is known, it is possible to recover the infinitesimal generators on a common dense domain, and the exponentiated fields have the advantage of being bounded. A more important difficulty arises from Haag's theorem. Although it is known that all representations of the canonical fields with a finite number of degrees of freedom are equivalent to the Fock representation, it is not so in the case of an infinite number of degrees of freedom, where there is an infinite number of inequivalent representations. Haag's theorem states that in a theory that has a space invariant vacuum, any representation that is equivalent to the Fock representation cannot describe anything but a free system. One is then faced with the choice of working with a representation that one does not know, or use a theory that is not space invariant.

It is this second procedure that will be used here. The system is taken to have a finite number of particles N in a box of finite volume V. The calculations are made in the Fock representation, and at the end N and V go to infinity, with the ratio $\bar{\rho} = N/V$ a fixed constant. This procedure is called the thermodynamic limit, and its existence has been extensively studied by Ruelle[9] in the case of interacting many-body systems. An important example of this method for the description of a free Bose gas at finite temperature in terms of exponentiated canonical fields can be found in Araki and Woods.[10]

It has been suggested by some authors[11] that physical theories might be expressed in terms of coordinates other than the canonical fields, and that by such substitution, one might be able to describe phenomena not previously covered by the canonical formalism.

One such set of coordinates are the so-called current fields, defined in terms of the canonical fields by

$$\rho(x) = a^*(x)a(x),$$

$$\mathbf{J}(x) = (1/2i)\{a^*(x)\nabla a(x) - [\nabla a^*(x)]a(x)\}.$$

In all that will follow, we will assume all masses to be 1. The smeared form of the operators is

$$\rho(f) = \int \rho(x)f(x)dx,$$

$$J(\mathbf{g}) = \int \mathbf{J}(x) \cdot \mathbf{g}(x)dx,$$

and the a's are either Fermi or Bose fields for spinless neutral particles. Since we know the Fock representation

for the canonical fields, we can write it for the currents. On $\mathfrak{H}_N$, the N-particle sector of Fock space,

$$\rho(f)\psi_N = \sum_{i=1}^{N} f(x_i)\psi_N, \tag{I. 1}$$

$$J(\mathbf{g})\psi_N = \frac{1}{2i}\sum_{i=1}^{N}[\mathbf{g}(x_i)\cdot\nabla_i + \nabla_i\cdot\mathbf{g}(x_i)]. \tag{I. 2}$$

The Fock representation for the currents is the same whether one starts with Fermi or Bose fields. From the commutation relations of the canonical fields, it is possible to compute the commutation relations of the currents,

$$[\rho(f),\rho(g)] = 0, \tag{I. 3}$$

$$[\rho(f),J(\mathbf{g})] = i\rho(\mathbf{g}\cdot\nabla f), \tag{I. 4}$$

$$[J(\mathbf{g}),J(\mathbf{h})] = iJ(\mathbf{h}\cdot\nabla\mathbf{g} - \mathbf{g}\cdot\nabla\mathbf{h}), \tag{I. 5}$$

irrespective of the statistics of the initial canonical fields. To stay in the spirit suggested by algebraic considerations, one then forgets about the existence of canonical fields, and considers only the polynomial algebra in ρ and J, subject to (I. 3) to (I. 5). It is then easy to see that Eqs. (I. 1) and (I. 2) define a representation of this algebra, which we will call the Fock representation of the current fields.

The same comments can be made about this representation that were made about the Fock representation of the canonical fields; it can describe fields that have only a finite number of degrees of freedom, whereas representations of physical interest are expected to have an infinite number of degrees of freedom, and the thermodynamic limit of the Fock representation can again be used to avoid this difficulty. On an N-particle sector of Fock space, the density operators are obviously bounded, but the currents J are not. Fortunately, a procedure analogous to the exponentiation of the canonical fields to obtain the Weyl groups is also available in the case of currents. Goldin[12] has shown that it is possible to consider the group of operators $e^{i\rho(f)}\,e^{iJ(\mathbf{g})}$ and that a knowledge of $\langle e^{i\rho(f)}\rangle$ alone is sufficient, coupled with an equation of continuity, to contain all the physical information of the system, and it is possible to recover the infinitesimal generators on a common dense domain in a Hilbert space. A convenient way to do this for the exponentiate values of the density operator is by functional differentiation:

$$\mathcal{L}(f) = \langle e^{i\rho(f)}\rangle,\quad \langle i\rho(x)\rangle = \frac{\delta}{\delta f(x)}\mathcal{L}(f)\Big|_{f=0}, \tag{I. 6}$$

$$i^2\langle\rho(x)\rho(y)\rangle = \frac{\delta^2}{\delta f(x)\,\delta f(y)}\mathcal{L}(f)\Big|_{f=0}. \tag{I. 7}$$

It is also to be noted that other representations are known, especially the functional representation of Grodnick and Sharp[11] which describes both Fermi and Bose statistics, and can be shown to be equivalent to ordinary Schrödinger quantum mechanics when applied to ordinary Fock space.

C. The Hamiltonian

It is in the functional representation that one of the problems of current theory is most evident. Written in terms of canonical fields, the Hamiltonian is a polynomial of the fields; expressed in terms of currents, it is a more complex expression given by

$$H(x) = \tfrac{1}{8}\int \mathbf{K}^*(x)\frac{1}{\rho(x)}\mathbf{K}(x)dx + \iint \rho(x)V(x-y)\rho(y)dxdy \tag{I. 8}$$

and

$$\mathbf{K}(x) = \nabla\rho(x) + 2i\,\mathbf{J}(x) \text{ (see Ref. 11).}$$

The free Hamiltonian density contains a term $1/\rho(x)$, which at first sight, is not an operator-valued distribution. Grodnick and Sharp, however, are able to show that, although $1/\rho(x)$ is meaningless, the expression $\mathbf{K}(x)^*\,1/\rho(x)\mathbf{K}(x)$ is a bona fide operator-valued distribution and that the Hamiltonian is well defined. We will take a different approach and consider the Hamiltonian defined through its commutation relation with the density operator. We will then see that, up to a point, it is possible to determine its form in the Fock representation.

To the algebra defined by (I. 3) to (I. 5) is added an operator H that defines the time translations as follows:

$$[H,A] = -i\dot{A},\quad \forall\, A\in\mathfrak{A}.$$

It is to be noted that $H\in\mathfrak{A}$, i.e., is not a polynomial of ρ's and J's, as can be seen from the functional representation. In particular, if $A=\rho(f)$,

$$[H,\rho(f)] = -i\frac{\partial\rho(f)}{\partial t}.$$

We now assume that an equation of continuity analogous to the equation satisfied in ordinary quantum mechanics is to hold between the ρ's and the J's,

$$\frac{\partial\rho(x)}{\partial t} + \nabla\cdot\mathbf{J}(x) = 0$$

or in smeared form,

$$\frac{\partial}{\partial t}\rho(f) = J(\nabla f). \tag{I. 9}$$

Substituting in (I. 9) we have

$$[H,\rho(f)] = -iJ(\nabla f), \tag{I. 10}$$

and this equation gives a constraint on the Hamiltonian. The Hamiltonian in the Fock representation must have the form

$$H = -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2 + H_I$$

and whatever H_I may be, it commutes with the ρ's. In the Fock representation, the interaction Hamiltonian can at most be a polynomial in the density operators.

In this work, we will take the free Hamiltonian to be

$$H = -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_i^2.$$

II. SYMMETRIC FUNCTIONS

This section is divided into two main parts. In the first one, we review, after MacMahon,[13] some of the principal functions one can construct that will be symmetric under any interchange of their arguments. The second part will deal with ways to compute powers of the trace

of an operator raised to some power, when this operator is not in diagonal form.

A. The *s*, *a* and *h* functions

Consider the M quantities $\alpha_1\alpha_2\ldots\alpha_M$. We wish to construct functions of these quantities that will remain invariant under any permutation of the α's. The simplest case one can write are the one-part symmetric functions, defined as

$$s_i = \sum_{j=1}^{M} (\alpha_j)^i. \tag{II. 1}$$

The next most complicated form is the symmetric function

$$a_s = \sum_{i_1\cdots i_s} \alpha_{i_1}\alpha_{i_2}\ldots\alpha_{i_s} \tag{II. 2}$$

and the sums run from 1 to M for each index, subject to the conditions $i_1 < i_2 < \ldots < i_s$.

One can easily see that the generating function for the a's is the polynomial

$$(1-\alpha_1 x)(1-\alpha_2 x)\ldots(1-\alpha_M x) = \sum_{l=1}^{M} x^l(-1)^l a_l.$$

Finally, define the homogeneous product sums h by

$$h_s = \sum_{i=1}^{M}(\alpha_i)^s + \sum_{i<j}(\alpha_i)^{s-1}\alpha_j + \sum_{i<j}(\alpha_i)^{s-2}\alpha_j^2 + \cdots + \sum_{i<j<l}^{1}(\alpha_i)^{s-3}\alpha_j\alpha_l + \cdots. \tag{II. 3}$$

From now on, we will take M to be infinite. All equations will be purely formal, and the important question of convergence will be discussed in detail at the end, in Sec. IV.

We now give some properties of the symmetric functions defined above.

$$\sum_i h_i x^i = \frac{1}{\sum_i (-1)^i a_i x^i} = \frac{1}{(1-\alpha_1 x)(1-\alpha_2 x)\cdots}, \tag{II. 4}$$

$$\sum_i (-1)^i a_i x^i = \exp\left(-\sum_{i=1}^{\infty}\frac{s_i x^i}{i}\right), \tag{II. 5}$$

$$\sum_{i=0}^{\infty} h_i x^i = \exp\left(\sum_{i=1}^{\infty}\frac{s_i x_i}{i}\right), \tag{II. 6}$$

$$h_n = \sum_{\{p\}}\left(\frac{s_1}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{s_2}{2}\right)^{p_2}\frac{1}{p_2!}\cdots, \tag{II. 7}$$

where $\sum_{\{p\}}$ means to sum over all values of the p's, subject to the condition

$$p_1 + 2p_2 + \cdots + np_n = n.$$

Similarly, we find

$$a_n = \sum_{\{p\}}(-1)^{i+\Sigma_i p_i}\left(\frac{s_1}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{s_2}{2}\right)^{p_2}\frac{1}{p_2!}\cdots. \tag{II. 8}$$

We can also express these functions in terms of an Hermitian operator A with eigenvalues α. We get

$$s_l = \sum_j (\alpha_j)^l = \mathrm{Tr}(A^l) = s_l(A).$$

Equations (II. 7) and (II. 8) can be written as

$$h_n(A) = \sum_{\{p\}}\left(\frac{\mathrm{Tr}A}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{\mathrm{Tr}(A^2)}{2}\right)^{p_2}\frac{1}{p_2!}\cdots, \tag{II. 9}$$

$$a_l(A) = \sum_{\{p\}}(-1)^{l+\Sigma p}\left(\frac{\mathrm{Tr}A}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{\mathrm{Tr}(A^2)}{2}\right)^{p_2}\frac{1}{p_2!}\cdots. \tag{II. 10}$$

From Eq. (II. 6), we get

$$\sum_i h_i(A)x^i = \det[I/(I-Ax)]. \tag{II. 11}$$

The generating function of $h(A)$ is then $\det(I-Ax)^{-1}$. From Eq. (II. 5),

$$\sum_i (-1)^i a_i(A)(-x)^i = \det(I+Ax), \tag{II. 12}$$

which is the generating function of $a(A)$.

It may be appropriate at this time to note that the condition for $\det(I+Ax)$ to exist is that Ax be of trace class, which is precisely the condition for the a's to be well defined. The same is also true for the h's. This in turn means that $\sum_i \alpha_i x < \infty$, where the α are the eigenvalues of A, and that we have $\alpha_i x < 1$. But this is also the condition for the expansion of $1/(1-\alpha_i x)$ in powers of x to be valid. When we discuss convergence, then, it will be sufficient to restrict ourselves to the final determinant, since its convergence insures the convergence of the other series used to obtain it.

For completeness, we include a property of the h functions that if we have two operators A and B and $A = xB$ for some scalar x, then

$$h_N(A) = x^N h_N(B), \quad a_N(A) = x^N a_N(B). \tag{II. 13}$$

Finally, we note that if Ax is of trace class, $\det(I+Ax)$ is finite. This implies

$$\lim_{N\to\infty} a_N(A) = 0$$

because

$$\det(I+Ax) = \sum_{l=0}^{\infty}(-1)^l a_l(A)x^l. \tag{II. 14}$$

Similarly,

$$\frac{1}{\det(I-Ax)} = \sum_{l=0}^{\infty} h_l(A)x^l,$$

and if x is not the inverse of one of the eigenvalues of A, this determinant is finite. In that case,

$$\lim_{N\to\infty} h_N(A) = 0.$$

B. Non-diagonal forms for *h* and *a* functions

As we have seen above, the h and a functions are relatively easy to compute when the eigenvalues of the operator are known. If this is not the case, Eq. (II. 9) expressing h as a sum of powers of the trace of different

powers of A is still true, but Eq. (II. 7) no longer holds; it has to be replaced by a sum over numbers with two indices, i.e., the matrix elements themselves.

Assume then that we have a quantity $f(i_1 \cdots i_s)$ that depends on s indices all running from 1 to infinity. We are given $\sum_{i_1 \ldots i_s} f(i_1 \ldots i_s)$ to evaluate. We seek to find an expression for this sum in terms of what will be called "restricted sums." A restricted sum over $i_1, i_2, i_3, i_4, \ldots, i_s$ is a sum over these indices where a condition like $i_1 < i_2 < i_3 < \cdots < i_s$ or "no two i's are equal" is imposed. We will find formulas when there are two and three indices. These will then be applied to the computation of some of the terms that appear in the expression for $h_2(A), h_3(A), a_2(A)$, and $a_3(A)$.

For two indices, we have to evaluate

$$\sum_{ij} f(i,j).$$

The relative values of the indices can only be

$$i = j, \quad i < j, \quad \text{or } i > j.$$

Then,

$$\sum_{ij} f(i,j) = \sum_i f(i,i) + \sum_{i<j} f(i,j) + \sum_{i>j} f(i,j), \qquad \text{(II. 15)}$$

which is equivalent to

$$\sum_i f(i,i) + \sum_{i \neq j} f(i,j).$$

By similar arguments, we find the following results for three indices:

$$\sum_{ijl} f(i,j,l) = \sum_i f(iii) + \sum_{i \neq l} f(iil) + \sum_{i \neq j} f(ijl) + \sum_{i \neq j \neq l} f(ijl) + \sum_{i \neq j} f(jii). \qquad \text{(II. 16)}$$

The same procedure can be extended to any number of indices; since we will only consider symmetric functions up to index three, it is enough to give the restricted sums up to three indices.

These two equations can be used to compute traces of powers of an operator not in diagonal form, or different powers of these traces.

We give some results that will be of use later:

$$\mathrm{Tr}A = \sum_i a_{ii}, \qquad \text{(II. 17)}$$

$$\mathrm{Tr}(A^2) = \sum_i a_{ii}^2 + \sum_{i \neq j} a_{ij} a_{ji}, \qquad \text{(II. 18)}$$

$$\mathrm{Tr}(A^3) = \sum_i a_{ii}^3 + 3 \sum_{i \neq j} a_{ii} a_{ji} a_{ij} + \sum_{i \neq j \neq l} a_{ij} a_{jl} a_{li}, \qquad \text{(II. 19)}$$

$$\mathrm{Tr}(A)\mathrm{Tr}(A^2) = \sum_l a_{ll}^3 + 2 \sum_{i \neq l} a_{ii} a_{il} a_{li} + \sum_{i \neq j} a_{ii} a_{jj}^2 + \sum_{i \neq j \neq l} a_{ii} a_{jl} a_{lj}, \qquad \text{(II. 20)}$$

$$(\mathrm{Tr}A)^2 = \sum a_{ii}^2 + \sum_{i \neq j} a_{ij} a_{ji}, \qquad \text{(II. 21)}$$

and

$$(\mathrm{Tr}A)^3 = \sum_i a_{ii}^3 + \sum_{i \neq j} a_{ii}^2 a_{jj} + \sum_{i \neq j \neq l} a_{ii} a_{jj} a_{ll}. \qquad \text{(II. 22)}$$

Since we will have to use Fourier transforms later, we will give here the convention that we will use for normalization. In a three-dimensional box of volume V, a complete orthonormal set of plane waves is

$$(1/\sqrt{V}) e^{-i\mathbf{k}\cdot\mathbf{x}}$$

The Fourier transform of the function $f(\mathbf{x})$ is given by

$$\tilde{f}(\mathbf{k}) = \int_V e^{-i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x}) d\mathbf{x},$$

and the inverse Fourier transform, if it exists, by

$$\tilde{f}(\mathbf{x}) = (1/V) \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \tilde{f}(\mathbf{k}).$$

This definition insures that if the volume of the box becomes infinite, and $f(\mathbf{x})$ is of sufficiently fast decrease at inifnity, both the Fourier transform and its inverse will exist. The completeness of this set of plane waves is expressed as usual by

$$\delta(\mathbf{x} - \mathbf{x}') = \frac{1}{V} \sum_k e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')},$$

which goes to $(2\Pi)^{-3} \int d\,\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}^1)}$ when the volume of the box becomes infinite:

$$\delta_{\mathbf{k},\mathbf{k}'} = \frac{1}{V} \int_V d\mathbf{x} e^{i\mathbf{x}\cdot(\mathbf{k}-\mathbf{k}')},$$

which becomes $\delta(\mathbf{k} - \mathbf{k}')$ in the infinite volume case.

If $K(\mathbf{x}, \mathbf{y})$ is the kernel of an integral transform of functions in the box, its Fourier transform will be given by

$$\tilde{K}(\mathbf{k}, \mathbf{k}') = \int_V e^{i\mathbf{k}\cdot\mathbf{x}} e^{-i\mathbf{k}'\cdot\mathbf{y}} K(\mathbf{x}, \mathbf{y}) d\mathbf{x} d\mathbf{y} \qquad \text{(II. 23)}$$

and the inverse Fourier transform by

$$K(\mathbf{x}, \mathbf{y}) = \frac{1}{V2} \sum_{\mathbf{k},\mathbf{k}_2} e^{-i\mathbf{k}_1\cdot\mathbf{x}} e^{i\mathbf{k}_2\cdot\mathbf{y}} \tilde{K}(\mathbf{k}_1, \mathbf{k}_2),$$

which will go to

$$\to \frac{1}{(2\Pi)^6} \int d\mathbf{k}_1 d\mathbf{k}_2 e^{i\mathbf{k}_1\cdot\mathbf{x}} e^{i\mathbf{k}_2\cdot\mathbf{y}} \tilde{K}(\mathbf{k}_1, \mathbf{k}_2)$$

in the limit of infinite volume.

III. FREE SYSTEMS IN THE BOX

We now turn to the task of computing the state of the exponentiated group of the current algebra describing a free system, first with Bose, then with Fermi statistics, for N particles in a box of finite volume V.

This state is obtained by taking a canonical average over a complete orthonormal basis spanning the vector space describing the N-particle system. This state will be referred to in what follows as the canonical state of the system.

A. The free Bose gas

We follow Messiah[14] and define a complete set of vectors in the occupation representation by $|n_1, n2, \cdots\rangle$ with $n1 + n2 + \cdots = N$. This vector describes a system of N particles, n_1 of which are in level k_1, n_2 in level k_2, etc. The statistics of the system are specified by a projection operator $E_{-(+)}$ for Fermi (Bose) statistics on the antisymmetric (symmetric) subspace of the space

spanned by $|n_1, n_2, \cdots\rangle$. Such a vector will be denoted by $E_+\,\Omega(N, V)$ in this first section that deals with bosons. It can be written

$$E_+\,\Omega(N, V) = \frac{N!}{n_1!n_2!\cdots V^N}\, E_+ e^{\{i[k_1(x_1+\cdots+x_{n_1})+k_2(x_{n_1+1},\cdots)+\cdots]\}}.$$

Such vectors form a complete orthonormal basis for all wave functions in the box, and

$$k_i = \Pi n_i/L$$

where L is the side of the box and n_i are integers.

The symmetric projection operator can be written as

$$E_+ = 1/N!\sum_{\Pi},$$

where $\pi = \begin{pmatrix} 1 & 2\ldots N \\ \Pi(1)\Pi(2)\ldots\Pi(N)\end{pmatrix}$

and the sum is carried over the $N!$ permutations of the N coordinates.

The Fock representation for the density operator $\rho(f)$ in the box is

$$\rho(f) = \sum_{i=1}^{N} f(x_i),$$

which implies

$$[\rho(f), E_+] = 0$$

and

$$\exp(i\rho(f)) = \exp\{i\,[f(x_1) + f(x_2) + \cdots + f(x_N)]\}.$$

In the canonical formalism, we have

$$\langle e^{i\rho(f)}\rangle_N(\beta) = \mathrm{Tr}e^{i\rho(f)}e^{(-\beta H_N)}/\mathrm{Tr}e^{(-\beta H_N)}.$$

This quantity is a linear, continuous, positive functional normalized to unity on the algebra of the exponentiated operators, i.e., it is a state on that algebra. From Sec. I, we know that it contains all the physical information on the system, and it is the quantity that we will compute in this chapter. Here, H is the N-particle Hamiltonian defined in Sec. I, i.e.,

$$H_N = -\tfrac{1}{2}\sum_{i=1}^{N}\nabla_{x_i}^2$$

We must first calculate $\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_N)}]$. Since the $\Omega(N, V)$ form a complete set, we will use them for that purpose, having in mind that H_N is diagonal in that representation, and commutes with E_+:

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_N)}] = \sum_{\{n\}}(E_+\Omega(V,N), e^{i\rho(f)}e^{(-\beta H_N)} \times E_+\Omega(V,N)),$$

where $\sum_{\{n\}}$ indicates a sum over all the indices n_i subject to the condition

$$N = \sum_i n_i.$$

Next, use the fact that

$$E_+^2 = E_+ = E_+^*, \qquad [E_+, \rho(f)] = 0 = [E_+, H_N],$$

to get

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_N)}] = \sum_{\{n\}}\int dx_1\ldots dx_N\, F(x_1)\ldots F(x_N) \times e^{-\beta(n_1k_1^2+n_1^2k_2^2+\cdots)/2}\frac{1}{n_1!n_2!\cdots V^N}\sum_{\Pi} \times \exp i\{k_1[(x_1 - x_{\Pi(1)}) + (x_2 - x_{\Pi(2)}) + \cdots + (x_{n_1} - x_{\Pi(n_1)})] + k_2[(x_{n_1+1} + x_{\Pi(n_1+1)}) + \cdots + (x_{n_2} - x_{\Pi(n_2)})] + k_3[\cdots] + \cdots\}, \quad \text{(III. 1)}$$

where

$$F(x) = e^{if(x)}.$$

We will now give the value of this sum when $N = 1, 2$, and 3:

$$N = 1:\ \mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_1)}] = \int_V \frac{F(x)}{V}\,dx\sum_k e^{(-\beta k^2/2)};$$

$$N = 2:\ \mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_2)}] = \int_V dx_1dx_2 \times\frac{F(x_1)F(x_2)}{V^2}\left(\sum_i e^{(-\beta k_i^2)} + \sum_{i<j} e^{[-\beta(k_i^2+k_j^2)/2} \times\{1 + e^{[i(k_i-k_j)(x_1-x_2)]}\}\right);$$

$$N = 3:\ \mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_3)}] = \int_V \frac{dx_1dx_2dx_3}{V^3}F(x_1)F(x_2)F(x_3) \times\left[\sum_i e^{(-3\beta k_i^2/2)} + \sum_{i\neq j} e^{[-\beta(2k_i^2+k_j^2)/2]} \times\{1 + e^{[i(k_i-k_j)(x_2-x_3)]} + e^{[i(k_i-k_j)(x_1-x_3)]}\} + \sum_{i<j<l} e^{[-\beta(k_i^2+k_j^2+k_l^2)/2]} \times(1 + e^{[i(k_i^2-k_j^2)(x_2-x_1)]} + e^{[i(k_j-k_l)(x_2-x_3)]} + e^{[i(k_i-k_l)(x_1-x_3)]} + e^{\{i[k_i(x_1-x_2)+k_j(x_2-x_3)+k_l(x_3-x_1)]\}} + e^{\{i[k_i(x_1-x_3)+k_j(x_2-x_1)+k_l(x_3-x_2)]\}}\right].$$

If we now define the Fourier transform of $F(x)$ as

$$\tilde{F}(k) = \int_V F(x)e^{-ikx}\,dx \quad \text{(III. 2)}$$

and the matrix elements a_{ij} as

$$a_{ij} = (1/V)\tilde{F}(k_i - k_j)e^{(-\beta k_j^2/2)}, \quad \text{(III. 3)}$$

we get

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_1)}] = \sum_i a_{ii}, \quad \text{(III. 4)}$$

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_2)}] = \sum_i a_{ii}^2 + \sum_{i<j}(a_{ii}a_{jj} + a_{ij}a_{ji}, \quad \text{(III. 5)}$$

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_3)}] = \sum_i a_{ii}^3 + \sum_{i\neq j}(a_{ii}^2a_{jj} + a_{ii}a_{ij}a_{ji} + a_{ii}a_{ji}a_{ij}) + \sum_{i<j<l}(a_{ii}a_{jj}a_{ll} + a_{ll}a_{ij}a_{ji} + a_{jj}a_{li}a_{il} + a_{ii}a_{jl}a_{lj} + a_{ij}a_{jl}a_{li} + a_{il}a_{lj}a_{ji}). \quad \text{(III. 6)}$$

Consider next the operator $A = \exp[if(x)]\exp(-\beta H)$ on one-particle space, where H is the usual one-particle free Hamiltonian.

Using the results of Sec. II whenever necessary, we see that

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_1)}] = h_1(A),$$

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_2)}] = h_2(A),$$

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_3)}] = h_3(A).$$

The generalization of these results is then obvious, and for N particles in the box,

$$\mathrm{Tr}(e^{i\rho(f)}e^{-\beta H_N}) = h_N(A),$$

where $A = e^{if(x)}e^{-\beta H}$ on one-particle wave functions in the box. From this, the expectation value for $e^{i\rho(x)}$ obtained by the canonical procedure, the canonical state, is

$$\langle e^{i\rho(f)}e^{(-\beta H_N)}\rangle = h_N(A(f))/h_N(A(0)). \qquad \text{(III. 7)}$$

This is the state for the representation of the exponentiated group of the current algebra corresponding to a free gas of N bosons in a box of volume V at temperature $\beta = 1/RT$.

This method is applied with the necessary modifications to the case of the Fermi system. The operator A is defined as in the case of bosons, and the state is found to be

$$\langle e^{i\rho(f)}e^{(-\beta H_N)}\rangle = \mathrm{Tr}e^{i\rho(f)}e^{(-\beta H_N)}/\mathrm{Tr}e^{(-\beta H_N)} = a_N(A(f))/a_N(A(0))$$

for N fermions in a box of volume V at temperature $T = 1/\beta k$.

IV. THE THERMODYNAMIC LIMIT

The states obtained in Sec. III by the use of the canonical ensemble are not suitable for our purpose, which is to get the thermodynamic limit for the system. That this is so can be seen if one expands $h_N(A)$ in terms of traces of the operator $A = e^{if(x)}e^{-\beta H}$.

In the box, we have

$$\mathrm{Tr}e^{if}e^{-\beta H} = \frac{1}{V}\sum_k \int dx e^{ikx}e^{if(x)}\exp(-\beta k^2/2)e^{-ikx} = \frac{1}{V}\int e^{if(x)}dx\sum_k \exp(-\beta k^2/2)$$

and is well-defined. lim. th. TrA, however, is seen to diverge like

$$\mathrm{Tr}A \to \frac{1}{(2\Pi)^3}\int d\mathbf{k}\, e^{(-\beta k^2)}\int_{V\to\infty} e^{if(x)}dx \to V,$$

which diverges because of the space integral. It might be argued that even though $h_N(A)$ diverges, the state is given by the ratio of two such functions, and might remain finite in the limit. This is partially true, but nevertheless leaves the canonical formalism somewhat incomplete in the limit. If we expand the state for the Bose system, for example (and the argument is the same in the Fermi case), in terms of traces, we have

$$\langle e^{i\rho(f)}\rangle_N(\beta) = \sum_{\{p\}}\left(\frac{\mathrm{Tr}A(f)}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{\mathrm{Tr}(A^2(f))}{2}\right)^{p_2}\frac{1}{p_2!}\cdots \times\overline{\sum_{\{p\}}\left(\frac{\mathrm{Tr}A(0)}{1}\right)^{p_1}\frac{1}{p_1!}\left(\frac{\mathrm{Tr}(A^2(0))}{2}\right)^{p_2}\frac{1}{p_2!}\cdots},$$

where $\sum_{\{p\}}$ runs over all p's subject to the condition

$$N = p_1 + 2p_2 + \cdots + Np_N.$$

One might then argue that dividing both the numerator and the denominator by

$$V^N = V^{p_1}\cdot V^{2p_2}\cdot V^{3p_3}\cdots V^{Np_N}$$

would change the operator A into A/V, and that the state would become

$$\langle e^{if(\rho)}\rangle_N(\beta) = h_N\left(\frac{A}{V}(f)\right)\Big/h_N\left(\frac{A}{V}(0)\right).$$

The trace

$$\mathrm{Tr}(A/V) = \frac{1}{V}\sum_k e^{(-\beta k^2)}\frac{1}{V}\int_V e^{if(x)}dx$$

would remain finite in the thermodynamic limit.

This line of reasoning, although perfectly correct, does not bring us any closer to the value of the thermodynamic limit of the state, however, because of Eq. (II. 4), which tells us that

$$\lim_{N\to\infty} h_N(A) = 0,$$

and instead of having an indetermination of the type ∞/∞, we have one of the type 0/0, which at this time, cannot be determined.

A. Grand canonical state for Bose and Fermi systems

The solution to this problem lies in the usual method of applying the grand canonical formalism. We will follow the procedure given in Reif.[15] Let $\langle e^{i\rho(f)}\rangle_N(\beta,\mu)$ denote the state for N particles in thebox of volume V at temperature $T = \frac{1}{k\beta}$ and chemical potential μ, where $\mu < 0$ in all that will follow. We know that

$$\langle e^{i\rho(f)}\rangle_N(\beta,\mu) = \mathrm{Tr}e^{\beta\mu\hat{N}}e^{i\rho(f)}e^{(-\beta H_N)}/\mathrm{Tr}e^{\beta\mu\hat{N}}e^{(-\beta H_N)}$$

where N is the total number of particle operator. In the occupation number representation, $\hat{N}$ is diagonal and has eigenvalues N, and commute with ρ and H_N. We have:

$$\mathrm{Tr}[e^{i\rho(f)}e^{(-\beta H_N)}e^{\beta\mu\hat{N}}] = \sum_{N=0}^{\infty}e^{\beta\mu N}\times\sum_{\{m\}}(E_\pm\Omega(N,V), e^{i\rho(f)}e^{(-\beta H_N)}E_\pm\Omega(N,V)),$$

where $\Omega(N,V)$ and $\sum_{\{n\}}$ have the same signification as before. The upper (lower) sign refers to Bose(Fermi) statistics.

For Bose statistics, the sum $\sum_{\{n\}}$ has already been calculated in Sec. III and found to be equal to $h_N(A)$. We have then

$$\mathrm{Tr}e^{i\rho(f)}e^{(-\beta H_N)}e^{\beta\mu\hat{N}} = \sum_{N=0}^{\infty}e^{\beta\mu N}h_N(A).$$

From Eq. (II. 18), this last sum is $\det[I/(I - e^{if(x)}e^{-\beta(H-\mu)})]$. The grand canonical state for the free Bose gas at temperature $T = 1/k\beta$ is then

$$\langle e^{i\rho(f)}\rangle_N(\beta,\mu) = \det[I - (e^{if(x)} - 1)/(e^{\beta(H-\mu)} - I)]^{-1}. \qquad \text{(IV. 1)}$$

For Fermi statistics, we get

$$\langle e^{i\rho(f)}\rangle_N(\beta,\mu) = \det[I + (e^{if(x)} - 1)/(e^{\beta(H-\mu)} + I)]\,. \quad \text{(IV. 2)}$$

Let

$$\langle e^{i\rho(f)}\rangle = \exp\{-[\mathrm{Tr}\,\log(I-K]\}$$

with

$$K(x,y) = (e^{if(x)} - 1)\frac{1}{V}\sum_k e^{ik(x-y)}\,1/(e^{[\beta(k^2-\mu)]} - 1)$$

and

$$G(k) = e^{if(x)} - 1.$$

Expanding the logarithm in power series, we take the functional derivative $\delta/\delta f$ of each term, and then let $f = 0$. Only the first term survives and gives

$$\bar\rho = \rho(0) = \frac{1}{V}\int\langle\rho(y)\rangle\,dy.$$

But

$$\rho(0) = (1/V)\sum_k (e^{[\beta(k^2-\mu)]} - 1)^{-1} = N/V$$

$$\Rightarrow N = \sum_k (e^{[\beta(k^2-\mu)]} - 1)^{-1} = \sum_k n(k). \quad \text{(IV. 3)}$$

At this stage, a few comments are in order.

(1) This equation is taken as the defining equation for μ in terms of the average density $\bar\rho$ and the temperature. The relation between μ and these variables is seen to be the same we would get for the ordinary chemical potential of statistical mechanics.

(2) The constraint equation will obviously be the same for the Fermi gas, with the $-$ sign of the denominator replaced by a $+$ sign.

(3) In statistical mechanics, the average number of particles in level k at temperature T is given by $n(k) = 1/\{\exp[\beta(k^2-\mu)] \pm 1\}$ and we have the condition that $\sum_k n(k) = N$. It is evident that this interpretation arises naturally here, and we will take this function $n(k)$ to be the average occupation number.

(4) In the Bose system, as T decreases, β increases and so must μ in order that the number of particles in the $k = 0$ state be small enough for the condition (IV. 3) to hold. When the temperature becomes low enough, μ becomes equal to 0, and a phase transition occurs. The calculation of the critical temperature is more easily done in the thermodynamic limit, and will be given in the section dealing with the condensed Bose system.

B. Convergence of the states in the box

It is now time to turn to the important question of the convergence of the sums we have used so far, in particular the final expressions for the states in the canonical and grand canonical formalisms.

In the canonical formalism in the box, the state is expressed as a finite sum of different powers of the trace of $e^{if(x)}e^{\beta(H-\mu)}$. This trace is

$$\mathrm{Tr}A = \sum_k \int_V dx\,\frac{1}{\sqrt{V}}\,e^{ikx}\,e^{if(x)}\,e^{(-\beta k^2)}\,\frac{e^{-ikx}}{\sqrt{V}}$$

$$= \frac{1}{V}\sum_k e^{(-\beta k^2)}\int_V e^{if(x)}dx.$$

Since $f(x)$ is well behaved in the box, the trace of A is finite, and for finite N and V, the canonical states are well defined for both the Bose and Fermi systems.

The states obtained from the grand canonical formalism can be expressed in Fredholm power series:

$$\det(I-K) = \sum_{l=0}^{\infty}\frac{(-1)^l}{l!}\int_V dx_1\cdots dx_l K\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix},$$

where $K(x,y)$ is the kernel for the transformation,

$$K\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix} = \begin{vmatrix} K(x_1x_1)\;K(x_1,x_2)\cdots K(x_1,x_l)\\ K(x_2,x_1)\;K(x_2,x_2)\cdots K(x_2,x_l)\\ \cdot\\ \cdot\\ \cdot\\ K(x_l,x_1)\;K(x_lx_2)\cdots K(x_lx_l)\end{vmatrix}.$$

If the integration domain V is finite, if $K(x,y)$ is finite in V, and $\int_V K(x,x)dx < \infty$, then the series is absolutely convergent. In our case, we have

$$|K(x,y)| \le \bar\rho(e^{if(x)} - 1),$$

and since the integration domain V is finite, the Fredholm series is absolutely convergent.

In the case of the Bose system, however, the state is

$$\langle e^{i\rho(f)}\rangle_N(\beta,\mu) = I/\det[I - (e^{if(x)} - 1)/(e^{\beta(H-\mu)} - I)],$$

and we must investigate the possibility that the denominator vanishes. We write the state

$$\mathcal{L}(f) = \det(I - e^{-\beta(H-\mu)})/\det(I - e^{if(x)}e^{-\beta(H-\mu)}),$$

and check that $\det(I - e^{if(x)}e^{-\beta(H-\mu)}) \neq 0$, i.e., that $e^{if(x)}e^{-\beta(H-\mu)}$ has no eigenvalue equal to 1.

It is well known that a Hermitian operator is positive if and only if all its eigenvalues are positive. This implies that $e^{-\beta(H-\mu)} > 0$ and also $I - e^{-\beta(H-\mu)} > 0$ for $\mu < 0$. We also note that the operator $e^{if(x)}$ is unitary. Then,

$$\|e^{if(x)}e^{-\beta(H-\mu)}\| \le \|e^{if(x)}\|\,\|e^{-\beta(H-\mu)}\| < 1.$$

But if λ is an eigenvalue of the operator A, we have

$$\|A\psi\| \le \|A\|\,\|\psi\| \quad \text{for all} \quad \psi \in \mathfrak{H},$$

and in particular, if ψ is an eigenvector,

$$\|A\psi\| = |\lambda|^2\|\psi\| \le \|A\|\,\|\psi\| \Rightarrow |\lambda|^2 \le \|A\|,$$

i.e., all the eigenvalues are bounded by the norm.

In our case, the norm of $e^{if(x)}e^{-\beta(H-\mu)}$ is strictly less than one, and all the eigenvalues are also strictly less than 1. The determinant $\det(I - e^{if(x)}e^{-\beta(H-\mu)})$ does not vanish, and the Bose state is not infinite in the box.

The grand canonical state in the box is given by an absolutely convergent series whose general term a_l is given by

$$(-1)^l\int_V dx_1\cdots dx_l\,K\begin{pmatrix}x_1\cdots\dot{x}_l\\ x_1\cdots x_l\end{pmatrix}$$

and

$$K\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix}=\det K_{ij},\quad K_{ij}=\frac{1}{V}F(x)\sum_k e^{ik(x_i-x_j)}n(k).$$

We note that a_l has an upper bound that is independent of V. In fact, from Hadamard's theorem,

$$\left|K\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix}\right|\leq (l^l)^{1/2}M^l,$$

with $M=K(0)$.

Then

$$a_l\leq[(-1)^l/l!](PM)^l(l^l)^{1/2},$$

with

$$P=\int_V|F(x)|\,dx\leq\int_{V\to\infty}|F(x)|\,dx=P'$$

$$\Rightarrow a_l\leq[(-1)^l/l!](P'M)(l^l)^{1/2}.$$

Because this upper bound is independent of V, we can take the term by term limit of the series in the box when V becomes infinite, and this will give the state in the thermodynamic limit ω,

where $\omega=\det(I\pm K_\pm)^{\pm1}$,

with

$$K_\pm(x,y)=F(x)\int_{V\to\infty}e^{ik(x-y)}\,n_\pm(k)dk$$

$$n_\pm(k)=1/(e^{\beta(k^2-\mu)}\pm1),$$

and where the + (−) sign refers to the Fermi (Bose) case.

C. The condensed Bose system

The range of temperatures for which Eq. (IV. 1) and (IV. 2) are valid has not been discussed so far; now that the states have been computed in the thermodynamic limit, we will see that such a discussion is necessary, and in the case of the Bose system, gives a criterion for the phase transition.

The criterion of validity of the states is

$$N=\sum_k 1/(e^{[\beta(k^2-\mu)]}\pm1),$$

which becomes in the thermodynamic limit,

$$\bar\rho=[1/(2\Pi)^3]\int d\mathbf{k}\{e^{[\beta(k^2-\mu)]}\pm1\}^{-1}.$$

For the Fermi system, this does not cause any problem, since the integrand can vary only between zero and one, as expected from the Pauli exclusion principle.

In the case of Bose statistics, however, the situation is quite different. As T decreases, i.e., as β increases, μ increases by becoming closer to zero. It will reach this value at a temperature T_0 given by

$$\bar\rho=\frac{1}{(2\Pi)^3}\int d\mathbf{k}\,\frac{1}{e^{[\beta(k^2-\mu)]}-1}\to\frac{1}{(2\Pi)^3}\int\frac{d\mathbf{k}}{e^{(\beta k^2)}-1}.$$

This last equation can be solved[16] for β and the ρ function. The temperature T_0 below which the condition $\mu<0$ is not possible any more is

$$T_0=(3.31\hbar/mk)(\bar\rho)^{2/3}\qquad\text{(IV.4)}$$

where m is the mass of the particle and k Boltzman's constant. The state (IV. 1) that describe the Bose system is then valid only for $T>T_0$.

The reason why the equation cannot be satisfied for $T<T_0$ is, of course, because particles crowd in the $E=0$ ground level in such large number that the constraint imposed on the physical system by (Eq. (IV. 3) can no longer be satisfied. One way out of this problem is the procedure used by Araki and Woods[10] to take into account this macroscopic occupation of the ground state. The occupation density $n(k)=[e^{(\beta k^2)}-1]^{-1}$ in the condensed state is replaced by

$$n(k)\to n_1(k)+N_0\delta_{k,0}\qquad\text{(IV.5)}$$

in the box, where $n_1(k)$ is a smooth function at $k=0$ and N_0/N is a finite fraction. We will show that if one makes such a transformation, the new state one obtains is well defined both in the box and in the thermodynamic limit. We will also see that if we let $N_0=N$, i.e., take a pure condensate at $T=0$, the state one gets is identical to the state that can be computed directly from a modified grand canonical formalism. We will also see that the thermodynamic limit of such a state is different from the thermodynamic limit of the state one can compute directly at $T=0$ in the case of the Bose system, but that they are equal for the Fermi system at zero degree.

For bosons,

$$\langle e^{i\rho(f)}\rangle_N(\beta,\mu)=\det[I-K(x,y)]^{-1},$$

$$K(x,y)=G(x)(1/V)\sum_k n(k)e^{ik(x-y)},$$

$$n(k)=\{e^{[\beta(k^2-\mu)}-1\}^{-1}.$$

If $\mu=0$, let $n(k)\to n_1(k)+N_0\delta_{k,0}$ and $N-N_0=\sum_k n_1(k)$ so that the condition $(1/V)\int_V\langle\rho(x)\rangle\,dx=N$ is still valid. Then,

$$K(x,y)=G(x)\bar\rho_0+\frac{G(x)}{V}\sum_k n_1(k)\,e^{ik(x-y)}$$

and

$$\bar\rho_0=\frac{N_0}{V},$$

$$\det(I-K)=\sum_{l=0}^{\infty}\frac{(-)^l}{l!}\int_V G(x_1)G(x_2)\cdots G(x_l)\times\rho\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix}dx_1\cdots dx_l,$$

$$\rho\begin{pmatrix}x_1\cdots x_l\\ x_1\cdots x_l\end{pmatrix}=\begin{vmatrix}\rho_1(x_1-x_1)+\bar\rho_0\cdots\rho_1(x_1-x_l)+\bar\rho_0\\ \rho_1(x_2-x_1)+\bar\rho_0\cdots\rho_1(x_2-x_l)+\bar\rho_0\\ \cdot\\ \cdot\\ \cdot\\ \rho_1(x_l-x_1)+\bar\rho_0\cdots\rho_1(x_l-x_l)+\bar\rho_0\end{vmatrix},$$

$$\rho_1(x-y)=\frac{1}{V}\sum_k n_1(k)\,e^{ik(x-y)}.$$

As before, we see that the elements of the determinants are bounded by $\bar{\rho}$ and the Fredholm series converges in the box. In the thermodynamic limit, the same argument used before will also apply here, and so will Hadamard's inequality. The series will also be uniformly convergent, and the substitution (IV. 5) in no way modifies the convergence properties of the series. The state will then still be given by Eq. (IV. 1), with the occupation density changed according to (IV. 5).

Next, we investigate the behavior of the state at $T = 0$, when all the particles are in the ground state. The occupation density then becomes

$$n(k) = N\delta_{k_1 0},$$

$$K(x, y) = G(x)\bar{\rho},$$

$$\det(I - K) = \sum_{l=0}^{\infty} \frac{(-)^l}{l!} \int dx_1 \cdots dx_l \, G(x_1) \cdots G(x_l) \times \begin{vmatrix} \bar{\rho} \cdots \bar{\rho} \\ \bar{\rho} \cdots \bar{\rho} \end{vmatrix}$$

$$= 1 - \bar{\rho} \int_V dx G(x),$$

all the other terms of the Fredholm series will vanish because they contain determinants with identical rows. The state is then

$$\langle e^{i\rho(f)} \rangle_N (T = 0, \mu = 0) = [1 - \bar{\rho} \int_V (e^{if(x)} - 1)dx)^{-1} \quad \text{(IV. 6)}$$

$$\text{lim. th.} \to (1 - \bar{\rho} \int (e^{if(x)} - 1)dx)^{-1}.$$

Next, we show that this answer is

(1) equal to the one we get from a direct computation of the state at $T = 0$ by use of the grand canonical formalism,

(2) is different from the state we get from use of the canonical formalism at $T = 0$.

Assume that the system of bosons is in contact with a reservoir with which it can exchange particles, but not energy, the temperature of the system and the reservoir being fixed at zero degree. We wish to compute the probability that the system will be in a quantum state specified by the set of quantum numbers r. In our case, this set is simply N, since the wave function of the ground state is

$$\psi = 1/\sqrt{V^N}.$$

Following Reif,[15] we have

$$P_N \propto e^{-\alpha N}. \quad \text{(IV. 7)}$$

The parameter α is a characteristic of the reservoir, but it can also be defined by the condition

$$\bar{N} = \sum_{N=0}^{\infty} N P_N / \sum_{N=0}^{\infty} P_N \quad \text{(IV. 8)}$$

when there is no reservoir and the system has $\bar{N}$ particles. We can compute $\langle e^{i\rho(f)} \rangle_{\bar{N}}(\alpha)$ at chemical potential α and for number of particle $\bar{N}$ in the usual way, i.e.,

$$\langle e^{i\rho(f)} \rangle_{\bar{N}}(\alpha) = \sum_{N=0}^{\infty} P_N \langle e^{i\rho(f)} \rangle_N / \sum_{N=0}^{\infty} P_N = (1 - \bar{\rho} \int_V (e^{if(x)} - 1)dx)^{-1},$$

which is exactly the result of Eq. (IV. 6). Note that even in the thermodynamic limit, this state is different from the state one gets from a direct calculation; in the box, the canonical state at zero degree can be computed directly, and we have

$$\mathcal{L}(f) = \int_V dx_1 \cdots dx_N \frac{e^{if(x_1)}}{V} \cdots \frac{e^{if(x_N)}}{V} = \left(\frac{1}{V} \int_V e^{if(x)} dx \right)^N$$

and

$$\text{lim. th. } \mathcal{L}(f) = \text{lim. th} \left(1 + \frac{1}{V} \int_V (e^{if(x)} - 1)dx \right)^N = \text{lim. th.} \left(1 + \frac{\bar{\rho}}{N} \int_V (e^{if(x)} - 1)dx \right)^N = \exp\bar{\rho} \int (e^{if(x)} - 1)dx$$

with the integral over all space. This state is obviously different from the grand canonical state at $T = 0$, except at low $\bar{\rho}$ where they coincide.

It is known[17] that the most general form for $\mathcal{L}(f)$ at zero degree is

$$\mathcal{L}(f) = \int \exp(\rho \int (e^{if(x)} - 1)dx) d\mu(\rho).$$

In our case, $d\mu(x) = (1/\bar{\rho})e^{-x/\bar{\rho}} dx$.

We see that it is necessary that $\bar{\rho}$ be positive for this measure to be well defined.

For physical reasons, we expect the thermodynamic limit of canonical states and grand canonical states to be equal. Since they are obviously not for the Bose system at zero degree, we may suspect that this anomaly is in some way connected to the presence of the condensate, If this assumption is correct, the Fermi system, which has no phase transition at low temperature, should have its canonical and grand canonical states converge to each other in the thermodynamic limit. This is what we proceed to show.

In the grand canonical formalism,

$$\mathcal{L}(f) = \det(I + K),$$

$$K(x, y) = G(x) \frac{1}{V} \sum_k e^{ik(x-y)} n(k)$$

$$n(k) = 1/\{\exp[\beta(k^2 - \mu)] + 1\} \quad \text{in the box.}$$

From Eq. (II. 23), we write the Fourier transform of K

$$K(k_1, k_2) = \int dx_1 dx_2 e^{ik_1 x} e^{(-ik_2 y)} K(x, y) = [-k_2 n/V] \hat{G}(k_1 - k_2)$$

with $\hat{G}(k) = \int_V G(x) dx e^{-ikx}$.

The determinant is then expressed in the momentum representation as

$$\det(I + K) = \sum_{l=0}^{\infty} \frac{1}{l!} \sum_{k_1 \ldots k_l} \frac{1}{V^l} n(k_1) n(k_2) \cdots \times n(k_l) G \begin{pmatrix} k_1 \cdots k_l \\ k_1 \cdots k_l \end{pmatrix}$$

with the usual notation, and in the thermodynamic limit, it equals

$$\sum_{l=0}^{\infty} \frac{1}{l!} \int \frac{d\mathbf{k}_1 \cdots d\mathbf{k}_l}{(2\Pi)^{3l}} n(k_1) \cdots n(k_l)\, G\begin{pmatrix} k_1 \cdots k_l \\ k_1 \cdots k_l \end{pmatrix}.$$

At $T = 0$, for fermions,

$$n(k) = 1 \quad \text{if} \quad k < k_F$$
$$= 0 \quad \text{if} \quad k > k_F,$$

$$\det(I + K) = \sum_{l=0}^{\infty} \frac{1}{l!} \int_{k_i < k_F} \frac{dk_1 \cdots dk_l}{(2\Pi)^{3l}}\, G\begin{pmatrix} k_1 \cdots k_l \\ k_1 \cdots k_l \end{pmatrix}, \quad \text{(IV. 9)}$$

where k_F is the Fermi level.

We will now use a direct method of computation without using the grand canonical formalism. Take a state vector at $T = 0$ to be

$$\psi = \sqrt{\frac{N!}{V^N}}\, \exp^{[i(k_1 x_1 + k_2 x_2 + \cdots + k_N x_N)]}.$$

The state

$$\langle e^{i\rho(f)} \rangle_N (T = 0) = (E_- \psi, e^{i\rho(f)} E_- \psi)$$
$$= \frac{1}{V^N} \int dx_1 \cdots dx_N\, F(x_1) \cdots F(x_N)$$
$$\times \sum_{\Pi} \sigma(\Pi) e^{\{i[k_1(x_1 - x_{\Pi(1)}) + k_2(x_2 - x_{\Pi(2)}) + \cdots + k_N(x_N - x_{\Pi(N)})]\}}$$

with $F(x) = e^{if(x)}$.

This is precisely equal to the determinant of a matrix whose elements

$$a_{ij} = \hat{F}(k_i - k_j) = \int_V e^{[-ix(k_i - k_j)]} e^{if(x)} dx,$$
$$\langle e^{i\rho(f)} \rangle_N = \det[I + \hat{G}(k_i - k_j)]. \quad \text{(IV. 10)}$$

The state computed from the grand canonical formalism (IV. 9) has the same form, but is of infinite dimension. Here, however, the determinant in the box is of finite size, of dimension $m \times m$ where m is the number of states below the Fermi level. If we take the thermodynamic limit, the size of the cells in k-space goes like $1/V$, and the determinant becomes of infinite dimension. We will follow the standard procedure outlined in Riesz and Nagy. Let h be the size of the unit cell in k-space, and m the size of the determinant. Then

$$\det(I + \lambda Kh) = 1 + \lambda h \sum_{l=1}^{m} K_{ii} + \frac{\lambda^2 h^2}{2!}$$
$$+ \sum_{i,j=1}^{m} \begin{vmatrix} K_{ii} & K_{ij} \\ K_{ji} & K_{jj} \end{vmatrix} + \cdots + \frac{\lambda^m h^m}{m!}$$
$$\times \sum_{i_1 \cdots i_m = 1}^{m} \begin{vmatrix} K_{i_1 i_1} & \cdots & K_{i_m i_m} \\ K_{i_m, i_1} & \cdots & K_{i_m, i_m} \end{vmatrix}$$

is a series expansion for a finite determinant. In the thermodynamic limit, $h \to 0$, and the series converges to the ordinary Fredholm series, the sums go into integrals over momenta, up to the Fermi level, and the state becomes equal to the state (IV. 9).

This result, then, seems to support the idea that the condensation is responsible for the fact that the canonical and grand canonical states of condensed Bose systems differ even in the thermodynamic limit. The rigorous proof that these two states should differ for any system that exhibit a phase transition is outside the scope of this work and of course a major problem in itself.

D. The Hamiltonian

In this section, we will show how the results obtained before can be used for practical calculations. A method for calculating the Hamiltonian density will be explained, and the calculation will be carried through for the grand canonical state of the Bose gas at finite temperature. From that point, the equations of ordinary thermodynamics could be derived, with all other equations of physical interest.

First, it is necessary to have an expression for functionals of the exponentiated current fields. We will proceed as in the case of the density fields. Let $j(\mathbf{g})$ be the current operator on one-particle Fock space. We can write

$$J(\mathbf{g}) = \sum_{i=1}^{N} j(\mathbf{g})(x_i),$$
$$j(\mathbf{g})(x_i) = \frac{1}{2i} [\nabla_i \cdot \mathbf{g}(x_i) + \mathbf{g} \cdot \nabla_i(x_i)]$$

on the N-particle sector of Fock space. When we compute the state in the box, we will have to evaluate

$$\mathrm{Tr}\, e^{iJ(\mathbf{g})} e^{[-\beta(H_N)]}.$$

On N-particle space, this trace for the Bose gas will be

$$\mathrm{Tr}(\Omega(N, V), e^{iJ(\mathbf{g})} e^{(-\beta H_N)} E_+ \Omega(N, V))$$
$$= \sum_{\{n\}} \int dx_1 \cdots dx_N\, e^{ij(\mathbf{g})(x_1)} \cdots e^{[ij(\mathbf{g})(x_N)]}$$
$$\times e^{[-\beta(n_1 k_1^2 + m_2 k_2^2 + \cdots)/2]}$$
$$\times \sum_{\Pi} e^{\{i[k_1(x_1 - x_{\Pi(1)}) + x_2 - x_{\Pi(2)}) + \cdots + x_{n_1} - x_{\Pi(n_1)}) + k_2(\ldots) + \cdots]\}},$$

where $e^{ij(\mathbf{g})(x_1)}$ is not a simple function of x_1 as was the case for the density operator, but is an operator acting only on the x_1 coordinate. The important point to note here is that the N-particle operator separates into the product of N one-particle operators. With this fact in mind, it is evident that the computation can be carried through exactly as in the case of the densities, and in the thermodynamic limit, the state will be

$$\langle e^{iJ(\mathbf{g})} \rangle (\beta, \mu) = \det[I - B(e^{\beta(H-\mu)} - I)^{-1}]^{-1},$$
$$B = e^{ij(\mathbf{g})} - I.$$

In fact, the state for any N-particle operator that will separate into a product will be expressible in this manner. Take, for example, and since it will be needed later, the operator

$$\langle e^{iJ(\mathbf{g})} e^{i\rho(f)} e^{iJ(\mathbf{h})} \rangle.$$

On the N-particle sector, we can write it as

$$\langle e^{iJ(\mathbf{g})} e^{i\rho(f)} e^{iJ(\mathbf{h})} \rangle = \det[I - C(e^{\beta(H-\mu)} - I)^{-1}]^{-1},$$
$$C = e^{ij(\mathbf{g})} e^{i\rho(f)} e^{ij(\mathbf{h})} - I.$$

As a last remark, note that any system where the wavefunction $\psi(x_1 \cdots x_N)$ can be decomposed into the product of N one-particle wave functions will yield a state of the form

$$\det(I \pm A)^{\pm 1}$$

when we use this procedure, A being equal to $(e^{if} - I)e^{-\beta H}$ with H the one-particle Hamiltonian.

As we have seen in the first chapter, the Hamiltonian is not a simple expression of the fields. For the free system,

$$H = \tfrac{1}{8}\int dx \mathbf{K}^*(x) \cdot [1/\rho(x)]\mathbf{K}(x), \quad \mathbf{K}(x) = \nabla\rho(x) + 2i\mathbf{J}(x).$$

The problem, of course, is the $1/\rho(x)$. Since we are interested in the expectation values of H, we have to calculate the matrix elements of $K^*(x)[1/\rho(x)]K(x)$. We follow (Ref. 17) for this calculation. Let

$$R_{ij}(f, x, y) = \langle K_i^*(x)\, e^{i\rho(f)} K_j(y)\rangle .$$

Formally, we have

$$e^{i\rho(f)}\frac{1}{\rho(x)} = \int_0^\infty e^{i\rho(f+it\delta_x)}\,dt,$$

where δ_x is a delta function at x so that $\rho(\delta_x) = \rho(x)$. Define

$$N_{ij}(f, x) = \int_0^\infty R_{ij}(f + it\,\delta_x, x, x)dt .$$

Then, we have

$$H = \sum_i N_{ii}(f, x)\Big|_{f=0}.$$

If we were to use delta functions for smearing, we would encounter terms like $e^{\rho(x)}$ which are not well defined. We can avoid this problem by smearing with

$$\delta_{m,x}(y) = \begin{cases} n^s, & |\mathbf{x} - \mathbf{y}| \le 1/2ms, \\ 0, & \text{otherwise}, \end{cases}$$

where s is the dimensionality of the space, then evaluate all distributions, and at the end let n go to infinity. There is no rigorous justification for this procedure except the fact that it will give the correct answer when applied to the free system at finite temperature.

We want to compute:

$$\begin{aligned}\langle K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})\rangle &= \langle e^{i\rho(f)}\{\rho(\nabla\cdot\mathbf{g})\rho(\nabla\cdot\mathbf{g}) \\ &+ 2\rho(\mathbf{g}\cdot\nabla(\nabla\cdot\mathbf{g})) + 2i\rho(\mathbf{g}\cdot\nabla f)\rho(\nabla\cdot\mathbf{g})\}\rangle \qquad \text{(IV. 11)} \\ &+ 4\langle J(\mathbf{g})e^{i\rho(f)}J(\mathbf{g})\rangle.\end{aligned}$$

If we are to test with $\delta_{n,x_0}(z)$, we might expect terms like $\delta(z - x_0 \pm 1/2^{ns})$ to appear in the final result. Consider the operator $K(\mathbf{f})$ on one-particle space. It is

$$K(\mathbf{f}) = 2\mathbf{f}\cdot\nabla.$$

When the test function is δ_{n,x_0}, this operator will not produce any delta functions at $x_0 \pm 1/2^{ns}$. But the expectation value we have to calculate is

$$\begin{aligned}&\langle K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})\rangle \\ &\quad = \mathrm{Tr}\,K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})e^{-\beta(H-\mu)}/\mathrm{Tr}\,e^{-\beta(H-\mu)}, \\ &\quad \mathrm{Tr}\,K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})e^{-\beta(H-\mu)} \\ &\quad = \sum_i (\psi_i, K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})e^{-\beta(H-\mu)}\psi_i) \\ &\quad = \sum_i (K(\mathbf{g})\psi_i, e^{i\rho(f)}K(\mathbf{g})e^{-\beta(H-\mu)}\psi_i),\end{aligned}$$

where the ψ_i are a suitable set of vectors in the Hilbert space.

The final expectation value cannot contain any terms of the form $\delta(z - x \pm 1/2^{ns})$; this fact will allow us to neglect such terms when they arise in the calculation of the matrix element, since we know that they have to cancel out in the end. We are left with

$$\langle K^*(\mathbf{g})e^{i\rho(f)}K(\mathbf{g})\rangle = 4\langle J(\mathbf{g})e^{i\rho(f)}J(\mathbf{g})\rangle,$$

where the δ-like terms are to be neglected.

We know that

$$\langle \mathbf{J}(x)e^{i\rho(f)}\mathbf{J}(y)\rangle = \frac{1}{i^2}\frac{\delta^2}{\delta g(x)\delta h(y)}\mathfrak{L}(f, g, h)\Big|_{g=h=0},$$

$$\begin{aligned}\mathfrak{L}(f, g, h) &= \langle e^{iJ(\mathbf{g})}e^{i\rho(f)}e^{iJ(h)}\rangle \\ &= \det(I - A)^{-1}, \\ A &= (e^{ij(g)}e^{i\rho(f)}e^{ij(h)} - 1)(e^{\beta(H-\mu)} - 1)^{-1}.\end{aligned}$$

Taking the required functional derivatives, evaluating them at $g = h = 0$, and smearing twice with the same function l, we have

$$\begin{aligned}&\int \frac{\delta^2}{\delta g(x)\delta h(y)}\det(I - A)^{-1}l(x)l(y)dxdy(z, z') \\ &\quad = \mathfrak{L}(f, 0, 0)\Big(\mathrm{Tr}(I - A)^{-1}\int dx\,\frac{\delta A}{\delta f(x)}\,l(x)\mathrm{Tr}(I - A)^{-1} \\ &\qquad \times \int dy\,\frac{\delta A}{\delta h(y)}\,l(y)dy + \mathrm{Tr}(I - A)^{-1} \\ &\qquad \times \int \frac{\delta A}{\delta g(x)}(I - A)^{-1}\frac{\delta A}{\delta h(y)}\,l(x)l(y)dydx + \mathrm{Tr}(I - A)^{-1} \\ &\qquad \times \int \frac{\delta^2 A}{\delta g(x)\delta h(y)}\,l(x)l(y)dxdy\Big) \qquad \text{(IV. 12)}\end{aligned}$$

with

$$\begin{aligned}\int \frac{\delta A}{\delta g(x)}l(x)dx(z, z') &= [l(z)\nabla_z + \nabla_z l(z)]e^{if(z)} \\ &\times (e^{\beta(H-\mu)} - 1)^{-1}(z, z')\int dxdy \\ &\times \frac{\delta^2 A}{\delta g(x)\delta h(y)}\,l(x)l(y)(z, z') \\ &= [l(z)\nabla_z + \nabla_z l(z)]e^{if(z)}[l(z)\nabla_z + \nabla_z l(z)] \\ &\times (e^{\beta(H-\mu)} - 1)^{-1}(z, z').\end{aligned}$$

We will now evaluate each term of Eq. (IV. 12) when $l(z) = \delta_{n,x_0}(z)$, then let $f \to f + it\,\delta_{n,x_0}$, integrate over t from zero to infinity, and let n go to infinity, in that order. But first we show that when we make the substitution $f \to f + it\,\delta_{n,x_0}$ the operators $[I - A(f)]^{-1}$ that appear in the three terms of Eq. (IV. 12) can be assumed to be changed by this substitution by at most a factor of order $1/n$.

Consider then

$$D = A(f + it\,\delta_{n,x_0}) - A(f)$$

and let

$$k_{n,x_0}(\mathbf{y}) = \begin{cases} 1, & |y - x_0| \le 1/2n, \\ 0, & \text{otherwise.} \end{cases}$$

We have

$$D(\mathbf{x}, \mathbf{x}^1) = (e^{-tn} - 1)K_{n,x_0}(\mathbf{x})e^{if(\mathbf{x})}(e^{\beta(H-\mu)} - 1)^{-1}(\mathbf{x}, \mathbf{x}^1),$$

and acting on some function h, we have

$$[Dh(\mathbf{x})] = (e^{-tn^3} - 1)K_n(\mathbf{x})e^{if(\mathbf{x})}\int (e^{\beta(H-\mu)} - 1)^{-1} \times (\mathbf{x}, \mathbf{y})h(\mathbf{y})d\mathbf{y}.$$

We see then that as n goes to infinity, D has an upper bound that will go to zero. It is important to remark here that the convergence of D to zero is uniform in t, i.e., that the upper bound on D is independent of t. This in turn will permit us to consider $(I - A)^{-1}$ to remain unchanged under the transformation $f \to f + i\delta_{n,x_0}$.

The third term of Eq. (IV. 12) is

$$\frac{1}{(2i)^2}\int (I - A)^{-1}(\mathbf{z}, \mathbf{z}')\,2\mathbf{n}\cdot\nabla_{\mathbf{z}'}e^{if(\mathbf{z}')}\,2\mathbf{n}\cdot\nabla_{\mathbf{z}'} \times (e^{\beta(H-\mu)} - 1)^{-1}(\mathbf{z}', \mathbf{z})d\mathbf{z}d\mathbf{z}',$$

where the smearing has been carried out as before, and the contribution from the end points of the test function have been neglected. We now let $f \to f + it\,\delta_{n,x_0}$ and do the t integral. We have

$$\lim_{n\to\infty}\frac{1(4)}{(2i)^2}\int_0^\infty dt\,\exp(-tn^3)n^6\int d\mathbf{z}\int_{|z'-x_0|\le 1/(2n)^3} d\mathbf{z}' \times (I - A)^{-1}(\mathbf{z}, \mathbf{z}')\cdot\nabla_{\mathbf{z}'}e^{if(\mathbf{z}')}\nabla_{\mathbf{z}'}(e^{\beta(H-\mu)} - 1)^{-1}(\mathbf{z}', \mathbf{z}).$$

The integration interval is of order $1/n^3$, and will cancel out one n^3. After taking $f = 0$, then $A = 0$, we have that it equals

$$-\nabla^2(e^{\beta(H-\mu)} - I)^{-1}(\mathbf{x}_0, \mathbf{x}_0).$$

A similar procedure applied to the other terms of Eq. (IV. 12) will show them to be of order $1/n^3$, and we have in the end,

$$H = \mathrm{Tr}[-\tfrac{1}{2}\nabla^2(e^{\beta(H-\mu)} - I)^{-1}],$$

which is the answer one would expect for the Hamiltonian of a free Bose gas at finite temperature.

One final remark is in order here. The operator $\mathbf{K}^*(x)[1/\rho(x)]\mathbf{K}(x)$ is well defined on a vector when $\mathbf{K}$ is "related" to ρ.[11]

In particular, $\mathbf{K}$ is related to ρ on Bose vectors, but not on Fermi vectors. This calculation, however, could have been done starting with the Fermi state, and we would obviously have arrived at the correct answer. It seems then that the relatedness of $\mathbf{K}$ to ρ is not such a necessary feature, and that the method exposed here could allow us to compute the Hamiltonian even for vector on which $\mathbf{K}$ is not related to ρ.

CONCLUSION

As a conclusion, we might note two facts. First, the method used here is sucessful mainly because we already know what the wavefunction for the N-particle system is, and that it separates into products of one-particle wavefunctions. We can therefore proceed in the same manner for any problem with these properties; in particular, the infinite system in an external field is simply given by the same expressions, with the operator H being the one particle Hamiltonian of the free particle in the external field.

The second remark stems from the first; we still have no indication as to how to treat a fully interacting system, where the N-particle wave-function will not have the simplifying properties of the free case. If, however, a series or iterative calculation can be devised, the states calculated here will be of use as a check of the zeroth order term of these new and so far use known methods.

ACKNOWLEDGMENTS

The author wishes to thank Dr. R. T. Powers and Dr. D. H. Sharp without whose help this work would have been far less complete, especially for their suggestion of the calculations on the Hamiltonian.

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Boson realization of the unitary symplectic group

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(Received 7 July 1972)

A realization of the Lie algebra of the unitary symplectic group is proposed in terms of boson operators. The existence of a noncompact orthogonal group, complementary to the symplectic one, is shown. The highest weight polynomial of an irreducible representation of the latter group is constructed with the help of the former.

1. INTRODUCTION

Since the pioneering work of Schwinger[1] on the $SU(2)$ group, it has proved very useful to realize the Lie algebras of the unitary group and of its subgroups in terms of boson creation and annihilation operators and their representation spaces as homogeneous polynomials in the creation operators. The advantage of such a picture is that the generators of the Lie algebras act as differential operators on the vectors of the representation spaces.

The unitary group[2,3] and its orthogonal subgroup[4] have been thoroughly analyzed along these lines. This resulted in applications to the evaluation of Wigner coefficients, fractional parentage coefficients, matrix elements of operators, etc.[2,5,6]

In this paper, we are concerned with the symplectic subgroup of the unitary group of even dimension, which is connected with the seniority classification of atomic and nuclear states.[7] In Sec. 2, we recall the group structure which underlies the boson realizations of the unitary and orthogonal groups. The extension to the symplectic group is straightforward and is given in Sec. 3. This enables us to prove in Sec. 4 some results on the irreducible representations (IR) and the Casimir operator of the symplectic group. Finally, we show in Sec. 5 how to build the highest weight polynomial (hwp) of an IR of the symplectic group.

2. BOSON REALIZATION OF THE UNITARY AND ORTHOGONAL GROUPS

Let η_i, $i = 1,\ldots,N$, be N independent boson creation operators and ξ_i, $i = 1,\ldots,N$, the corresponding annihilation operators. They satisfy the commutation relations

$$[\eta_i,\eta_j] = [\xi_i,\xi_j] = 0, \qquad [\xi_i,\eta_j] = \delta_{ij}. \tag{2.1}$$

The problem amounts to writing the generators of the Lie algebra of the group under consideration, in terms of these operators, and then finding the sets of linearly independent polynomials in the creation operators

$$P(\eta_i) = P(\eta_1,\eta_2,\ldots,\eta_N) \tag{2.2}$$

forming bases for the IR of the group. From (2.1), we see that when applied to the polynomials (2.2), the annihilation operators can be interpreted as differential operators, i.e.,

$$\xi_i = \frac{\partial}{\partial\eta_i}. \tag{2.3}$$

We consider the $N(2N+1)$ bilinear operators

$$\mathbf{H}_i = \tfrac{1}{2}(\eta_i\xi_i + \xi_i\eta_i) \equiv \mathbf{C}_{ii} + \tfrac{1}{2}, \qquad i = 1,\ldots,N, \tag{2.4a}$$

$$\eta_i\xi_j \equiv \mathbf{C}_{ij}, \qquad i \neq j,\ i,j = 1,\ldots,N, \tag{2.4b}$$

$$\eta_i\eta_j \equiv \mathbf{D}^{\dagger}_{ij}, \qquad i \leq j = 1,\ldots,N, \tag{2.4c}$$

$$\xi_i\xi_j \equiv \mathbf{D}_{ij}, \qquad i \leq j = 1,\ldots,N. \tag{2.4d}$$

From (2.1), they close under commutation. It is well known[8,9] that they are the generators of a (noncompact) symplectic group in $2N$ dimensions, $\mathbf{Sp}(2N)$ (the dynamical group of the N-dimensional harmonic oscillator). The operators $\mathbf{C}_{ij}$, $i,j = 1,\ldots,N$, which form a close set under commutation, are the generators of the subgroup $\mathbf{U}(N)$ of the group $\mathbf{Sp}(2N)$.

In what follows, it is useful to replace the i index by a pair of indices μ,s, which take the values $\mu = 1,\ldots,q$ and $s = 1,\ldots,n$, respectively, with $N = nq$. With this change, we are able to find subgroups of the group $\mathbf{U}(nq)$. Contracting the operators $\mathbf{C}_{\mu s,\nu t}$ with respect to index s, we obtain the operators

$$\mathcal{C}_{\mu\nu} \equiv \sum_{s=1}^{n} \mathbf{C}_{\mu s,\nu s}, \qquad \mu,\nu = 1,\ldots,q, \tag{2.5}$$

which are the generators of a subgroup $\mathfrak{U}(q)$ of the group $\mathbf{U}(nq)$. We can also contract the operators $\mathbf{C}_{\mu s,\nu t}$ with respect to index μ, obtaining the operators

$$C_{st} \equiv \sum_{\mu=1}^{q} \mathbf{C}_{\mu s,\mu t}, \qquad s,t = 1,\ldots,n, \tag{2.6}$$

which are the generators of a subgroup $U(n)$ of the group $\mathbf{U}(nq)$. Moreover the operators (2.5) and (2.6) commute with one another, so that we can form the direct product of the groups $\mathfrak{U}(q)$ and $U(n)$. Thus we have the following chain of groups:

$$\mathbf{Sp}(2nq) \supset \mathbf{U}(nq) \supset \mathfrak{U}(q) \times U(n). \tag{2.7}$$

The operators (2.5), with definitions (2.4a) and (2.4b), constitute a boson realization of the Lie algebra of the unitary group $\mathfrak{U}(q)$. The operators with $\mu = \nu$, $\mu < \nu$, and $\mu > \nu$ are the weight, raising and lowering generators of the group $\mathfrak{U}(q)$, respectively. The usefulness of the group chain (2.7) appears when one looks for polynomial bases of the IR of the group $\mathfrak{U}(q)$.

The set of all polynomials in the creation operators (2.2) belong to one of two (infinite-dimensional) IR of the group $\mathbf{Sp}(2nq)$.[9] The polynomials of even (odd) degree form an IR characterized by the eigenvalues of the nq weight generators (2.4a) corresponding to the minimum weight polynomial $1\,(\eta_{nq})$, i.e.,

$$[\tfrac{1}{2}\tfrac{1}{2}\cdots\tfrac{1}{2}] = [(\tfrac{1}{2})^{nq}] \quad \text{or} \quad [\tfrac{1}{2}\tfrac{1}{2}\cdots\tfrac{1}{2}\tfrac{3}{2}] = [(\tfrac{1}{2})^{nq-1}\tfrac{3}{2}]. \tag{2.8}$$

When restricted to the group $\mathbf{U}(nq)$, each IR of the group $\mathbf{Sp}(2nq)$ decomposes into IR of the subgroup characterized by the partitions

$$[\nu 0^{nq-1}] \quad \nu = 0,2,4,\cdots \text{ or } 1,3,5,\ldots, \tag{2.9}$$

according as the degree is even or odd. The hwp of

these IR's are given by η^{ν}_{11}.

As they are completely symmetrical, the IR (2.9) of the group $\mathbf{U}(nq)$ decompose into direct products of IR of the groups $\mathfrak{U}(q)$ and $U(n)$ characterized by the same partition of ν:

$$[\lambda_1\lambda_2\cdots\lambda_p], \quad \sum_{\mu=1}^{p}\lambda_\mu = \nu, \tag{2.10}$$

into p parts, p being given by

$$p = \min(q,n). \tag{2.11}$$

Thus there is a one-to-one correspondence between the IR of the subgroups $\mathfrak{U}(q)$ and $U(n)$ contained in a given IR of $\mathbf{Sp}(2nq)$ or $\mathbf{U}(nq)$. Following Ref. 10, both subgroups are said to be complementary within the IR of the larger group $\mathbf{Sp}(2nq)$ or $\mathbf{U}(nq)$.

The complementarity of the groups $\mathfrak{U}(q)$ and $\mathbf{U}(n)$ leads to the following important property, first noted by Moshinsky:[2] The linearly independent polynomials in the creation operators of the type (2.2) that satisfy the equations

$$C_{ss}P = \lambda_s P, \qquad s = 1,\ldots,n, \tag{2.12a}$$

$$C_{st}P = 0, \qquad s < t = 2,\ldots,n, \tag{2.12b}$$

form a basis for an IR of $\mathfrak{U}(q)$ characterized by the partition $[\lambda_1\lambda_2\cdots\lambda_p]$ (and $\lambda_{p+1} = \cdots = \lambda_n = 0$ if $n > q$). Note that the operators C_{ss} and C_{st} $(s<t)$ are the weight and raising generators of the complementary group $U(n)$, respectively. The hwp $\mathbf{P}$ of the IR of $\mathfrak{U}(q)$ is given by the simultaneous solution of Eqs. (2.12) and

$$\mathcal{C}_{\mu\nu}\mathbf{P} = 0, \quad \mu < \nu = 2,\ldots,q. \tag{2.13}$$

In order to get all possible q-row IR of the group $\mathfrak{U}(q)$, it is necessary by (2.11) that $n \geq q$. By taking $n = q$, the group chain (2.7) becomes

$$\begin{array}{lllll}\mathbf{Sp}(2q^2) \supset & \mathbf{U}(q^2) \supset & \mathfrak{U}(q) & \times & U(q),\\ [(\frac{1}{2})^{q^2}] & & & & \\ [(\frac{1}{2})^{q^2-1}\tfrac{3}{2}]\,[\nu] & & [\lambda_1\lambda_2\cdots\lambda_q] & & [\lambda_1\lambda_2\cdots\lambda_q],\end{array} \tag{2.14}$$

where we show under each group the IR to which it corresponds.

The solution of Eqs. (2.12), with $n = q$, can be given[2] in terms of the determinants

$$\Delta^{s_1 s_2\cdots s_r}_{\mu_1\mu_2\cdots\mu_r} = \sum_{\mathcal{P}}[(-1)^{\mathcal{P}}\,\mathcal{P}\,\eta_{\mu_1 s_1}\eta_{\mu_2 s_2}\cdots\eta_{\mu_r s_r}], \quad r = 1,\ldots,q, \tag{2.15}$$

where $\mathcal{P}$ stands for a permutation of $s_1, s_2, \ldots, s_r$, as

$$P = (\Delta^1_1)^{\lambda_1-\lambda_2}(\Delta^{12}_{12})^{\lambda_2-\lambda_3}\cdots(\Delta^{12\cdots q-1}_{12\cdots q-1})^{\lambda_{q-1}-\lambda_q} \times (\Delta^{12\cdots q}_{12\cdots q})^{\lambda_q} Z\left(\frac{\Delta^1_\mu}{\Delta^1_1}, \frac{\Delta^{12}_{1\mu}}{\Delta^{12}_{12}}, \ldots, \frac{\Delta^{12\cdots q-1}_{12\cdots\mu}}{\Delta^{12\cdots q-1}_{12\cdots q-1}}\right), \tag{2.16}$$

where Z is an arbitrary polynomial in the ratios indicated, subject only to the condition that P should be a polynomial in $\eta_{\mu s}$. The hwp $\mathbf{P}$ corresponds to

$$Z = 1. \tag{2.17}$$

We turn now to the boson realization of the orthogonal group $\mathcal{O}(q)$. To write it easily, let us first change index μ $(\mu = 1,\ldots,q)$ into a new index m, which takes the values

$$m = -l, -l+1, \ldots, -1, 0, 1, \ldots, l-1, l \tag{2.18a}$$

for $q = 2l+1$ odd, and

$$m = -l, -l+1, \ldots, -1, 1, \ldots, l-1, l \tag{2.18b}$$

for $q = 2l$ even (l is here any integer $l = 1, 2, \cdots$). A subset of the generators $\mathcal{C}_{mm'}$ of the group $\mathfrak{U}(q)$, given by

$$\Lambda_{mm'} = \mathcal{C}_{mm'} - (-1)^{m+m'}\mathcal{C}_{-m',-m}, \tag{2.19}$$

is closed under commutation:

$$[\Lambda_{mm'}, \Lambda_{m''m'''}] = \delta_{m'm''}\Lambda_{mm'''} - \delta_{mm'''}\Lambda_{m''m'} + (-1)^{m+m'''}\delta_{m',-m'''}\Lambda_{m'',-m} - (-1)^{m'+m''}\delta_{m,-m''}\Lambda_{-m',m'''}, \tag{2.20}$$

and is the set of generators of the subgroup $\mathcal{O}(q)$ of the group $\mathfrak{U}(q)$.[6] The weight, raising, and lowering generators are the operators with $m = m'$, $m > m' > -m$, and $m' > m > -m'$, respectively.

It is possible to build, within the group $\mathbf{Sp}(2nq)$, a group which plays the same role with respect to $\mathcal{O}(q)$ as the group $U(n)$ with respect to $\mathfrak{U}(q)$. Indeed the operators

$$H_s = \sum_m \mathbf{H}_{ms,ms} = C_{ss} + \tfrac{1}{2}q = \sum_m \eta_{ms}\xi_{ms} + \tfrac{1}{2}q, \qquad s = 1,\ldots,n, \tag{2.21a}$$

$$C_{st} = \sum_m \eta_{ms}\xi_{mt}, \quad s \neq t, \; s,t = 1,\ldots,n, \tag{2.21b}$$

$$D^{+}_{st} = \sum_m (-1)^{l-m}\mathbf{D}^{+}_{ms,-mt} = \sum_m (-1)^{l-m}\eta_{ms}\eta_{-mt}, \qquad s \leq t = 1,\ldots,n, \tag{2.21c}$$

$$D_{st} = \sum_m (-1)^{l-m}\mathbf{D}_{ms,-mt} = \sum_m (-1)^{l-m}\xi_{ms}\xi_{-mt}, \qquad s \leq t = 1,\ldots,n, \tag{2.21d}$$

are closed under commutation and are the generators of a (noncompact) subgroup $Sp(2n)$ of $\mathbf{Sp}(2nq)$.[9] Moreover they commute with the generators (2.19) of $\mathcal{O}(q)$. We have, therefore, instead of (2.7), the following chain of groups:[9]

$$\mathbf{Sp}(2nq) \supset \mathcal{O}(q) \times Sp(2n), \tag{2.22}$$

where $\mathcal{O}(q) \subset \mathfrak{U}(q)$ and $Sp(2n) \supset U(n)$.

As was shown by Chacón,[4] the IR of the groups $\mathcal{O}(q)$ and $Sp(2n)$ contained in an IR (2.8) of $\mathbf{Sp}(2nq)$ are characterized by the same partition

$$[\mu_1\mu_2\cdots\mu_r] \tag{2.23}$$

into r parts, r being given by

$$r = \min(l,n). \tag{2.24}$$

Thus the groups $\mathcal{O}(q)$ and $Sp(2n)$ are complementary within a given IR of $\mathbf{Sp}(2nq)$.

The complementarity of $\mathcal{O}(q)$ and $Sp(2n)$ leads to the following property, which was proved by Chacón:[4] The linearly independent polynomials in the creation operators of the type (2.2) that satisfy the equations

$$C_{ss}P = \mu_s P, \qquad s = 1,\ldots,n, \tag{2.25a}$$

$$C_{st}P = 0, \qquad s < t = 2,\ldots,n, \tag{2.25b}$$

$$D_{st}P = 0, \qquad s \leqslant t = 1,\ldots,n, \tag{2.25c}$$

form a basis for an IR of $\mathcal{O}(q)$ characterized by the partition $[\mu_1\mu_2\cdots\mu_r]$ (and $\mu_{r+1} = \cdots = \mu_n$ if $n > l$). Note that they are those polynomials which are of highest weight with respect to the subgroup $U(n)$ of $Sp(2n)$ and at the same time contain the minimum possible number of creation operators. The hwp $\mathbf{P}$ of the IR of $\mathcal{O}(q)$ is given by the simultaneous solution of Eqs. (2.25) and

$$\Lambda_{mm'}\,\mathbf{P} = 0, \qquad m > m' > -m. \tag{2.26}$$

In order to get all possible l-row IR of the group $\mathcal{O}(q)$, it is necessary by (2.24) that $n \geqslant l$. By taking $n = l$, the group chain (2.22) becomes

$$\begin{matrix}\mathbf{Sp}(2l(2l+1)) \supset \mathcal{O}(2l+1) \times Sp(2l), \\ [(\frac{1}{2})^{l(2l+1)}] \qquad [\mu_1\mu_2\cdots\mu_l][\mu_1\mu_2\cdots\mu_l], \\ [(\frac{1}{2})^{l(2l+1)-1}\tfrac{3}{2}]\end{matrix} \tag{2.27a}$$

or

$$\begin{matrix}\mathbf{Sp}(4l^2) \supset \mathcal{O}(2l) \times Sp(2l), \\ [(\frac{1}{2})^{2l^2}] \qquad [\mu_1\mu_2\cdots\mu_l]\,[\mu_1\mu_2\cdots\mu_l], \\ [(\frac{1}{2})^{2l^2-1}\tfrac{3}{2}]\end{matrix} \tag{2.27b}$$

following q is odd or even. Under each group we show the IR to which it corresponds.

The solution of Eqs. (2.25) and (2.26), with $n = l$, is[4]

$$\mathbf{P} = (\Delta_l^{1})^{\mu_1-\mu_2}(\Delta_{l\,l-1}^{1\;2})^{\mu_2-\mu_3}\cdots(\Delta_{l\,l-1\cdots 2}^{1\;2\cdots l-1})^{\mu_{l-1}-\mu_l} \times (\Delta_{l\,l-1\cdots 1}^{1\;2\cdots l})^{\mu_l}, \tag{2.28}$$

where the determinants $\Delta_{m_1m_2\cdots m_r}^{s_1s_2\cdots s_r}$ are defined as in (2.15).

We proceed now to extend the analysis developed in this section to the symplectic subgroup of the unitary group.

3. THE SYMPLECTIC GROUP AND ITS ORTHOGONAL COMPLEMENTARY GROUP

For q even, the unitary group $\mathcal{U}(q)$ has the symplectic group $\mathcal{S}p(q)$ among its subgroups. To get a boson realization of the latter, it is useful to introduce new notations as follows: q is set equal to $2j+1$, where j is any half-integer ($j = \frac{1}{2}, \frac{3}{2}, \cdots$), and index μ ($\mu = 1, 2, \ldots, 2j+1$) is changed into a new index m, which takes the values

$$m = -j, -j+1, \ldots, -\tfrac{1}{2}, \tfrac{1}{2}, \ldots, j-1, j. \tag{3.1}$$

Let us consider the subset of the generators $\mathcal{C}_{mm'}$ of the group $\mathcal{U}(q)$, given by

$$\Lambda_{mm'} = \mathcal{C}_{mm'} + (-1)^{m+m'}\mathcal{C}_{-m',-m}. \tag{3.2}$$

They satisfy the relations

$$\Lambda^{+}_{mm'} = \Lambda_{m'm}, \tag{3.3}$$

$$\Lambda_{-m',-m} = (-1)^{m+m'}\Lambda_{mm'}, \tag{3.4}$$

and are closed under commutation, the commutation relations being identical to Eqs. (2.20).

From (3.4), the operators $\Lambda_{mm'}$ ($m, m' = -j, \ldots, j$) are not independent. We can take as independent operators

$$\Lambda_{mm} \quad m > 0, \tag{3.5a}$$

$$\Lambda_{mm'} \quad m > m' \geqslant -m, \tag{3.5b}$$

$$\Lambda_{m'm} \quad m > m' \geqslant -m. \tag{3.5c}$$

From (2.20), it is easy to see that they are the weight, raising, and lowering generators of the subgroup $\mathcal{S}p(q)$ of $\mathcal{U}(q)$, respectively. The different elements of (3.5b) correspond to the following root vectors:

$$\begin{matrix}\Lambda_{mm'} & m > m' > 0, & e_{j-m+1} - e_{j-m'+1}, \\ \Lambda_{mm'} & m > 0 > m' > -m, & e_{j-m+1} + e_{j-|m'|+1}, \\ \Lambda_{m-m} & m > 0, & 2e_{j-m+1},\end{matrix} \tag{3.6}$$

and those of (3.5c) to

$$\begin{matrix}\Lambda_{m'm} & m > m' > 0, & -e_{j-m+1} + e_{j-m'+1}, \\ \Lambda_{m'm} & m > 0 > m' > -m, & -e_{j-m+1} - e_{j-|m'|+1}, \\ \Lambda_{-mm} & m > 0, & -2e_{j-m+1}.\end{matrix} \tag{3.7}$$

Within the group $\mathbf{Sp}(2nq)$, it is possible to find a group which plays the same role with respect to $\mathcal{S}p(q)$ as the groups $U(n)$ and $Sp(2n)$ with respect to $\mathcal{U}(q)$ and $\mathcal{O}(q)$, respectively. By analogy with Eqs. (2.21), we build the operators

$$H_s = \sum_m \mathbf{H}_{ms,ms} = C_{ss} + \tfrac{1}{2}q = \sum_m \eta_{ms}\xi_{ms} + \tfrac{1}{2}q, \qquad s = 1,\ldots,n, \tag{3.8a}$$

$$C_{st} = \sum_m \eta_{ms}\xi_{mt}, \qquad s \neq t,\ s,t = 1,\ldots,n, \tag{3.8b}$$

$$D^{+}_{st} = \sum_m (-1)^{j-m}\mathbf{D}^{+}_{ms,-mt} = \sum_m (-1)^{j-m}\eta_{ms}\eta_{-mt}, \qquad s < t = 2,\ldots n, \tag{3.8c}$$

$$D_{st} = \sum_m (-1)^{j-m}\mathbf{D}_{ms,-mt} = \sum_m (-1)^{j-m}\xi_{ms}\xi_{-mt}, \qquad s < t = 2,\ldots,n, \tag{3.8d}$$

where the summations are taken over the values (3.1). The operators D^{+}_{st} and D_{st} are antisymmetrical with respect to s and t, so that the restriction of s and t to the values shown in (3.8c) and (3.8d) ensures the linear independence of the corresponding operators.

The operators (3.8) are closed under commutation and are the generators of a (noncompact) orthogonal group $O(2n)$. The weight generators are the operators (3.8a). The raising and lowering generators with their corresponding root vectors are

$$\begin{matrix}C_{st} & s < t = 2,\ldots,n, & e_s - e_t, \\ D^{+}_{st} & s < t = 2,\ldots,n, & e_s + e_t,\end{matrix} \tag{3.9}$$

and

$$\begin{aligned} &C_{ts} \quad s<t=2,\ldots,n, \quad -e_s+e_t, \\ &D_{st} \quad s<t=2,\ldots,n, \quad -e_s-e_t, \end{aligned} \tag{3.10}$$

respectively. Moreover all the operators (3.8) commute with the generators (3.2) of $Sp(q)$, so that we can form the direct product of the groups $Sp(q)$ and $O(2n)$. We get, therefore, the following chain of groups:

$$\mathbf{Sp}(2nq) \supset Sp(q) \times O(2n), \qquad q = 2j+1. \tag{3.11}$$

We are now going to show that the IR of the groups $Sp(q)$ and $O(2n)$ contained in an IR (2.8) of $\mathbf{Sp}(2nq)$ are characterized by the same partition

$$[\mu_1\mu_2\cdots\mu_u] \tag{3.12}$$

into u parts, u being given by

$$u = \min(j+\tfrac{1}{2}, n). \tag{3.13}$$

The groups $Sp(q)$ and $O(2n)$ are thus complementary within a given IR of $\mathbf{Sp}(2nq)$.

More precisely, we are going to prove the following property: The linearly independent polynomials in the creation operators of the type (2.2) that satisfy the equations

$$C_{ss}P = \mu_s P, \qquad s=1,\ldots,n, \tag{3.14a}$$

$$C_{st}P = 0, \qquad s<t=2,\ldots,n, \tag{3.14b}$$

$$D_{st}P = 0, \qquad s<t=2,\ldots,n, \tag{3.14c}$$

form a basis for an IR of $Sp(q)$ characterized by the partition $[\mu_1\mu_2\cdots\mu_u]$ (and $\mu_{u+1}=\cdots=\mu_n=0$ if $n>j+\frac{1}{2}$). Note that they are those polynomials which are of highest weight with respect to the subgroup $U(n)$ of $O(2n)$ and at the same time contain the minimum possible number of creation operators.

In order to get all possible $(j+\frac{1}{2})$ — row IR of the group $Sp(q)$, it is necessary by (3.13) that $n \geq j+\frac{1}{2}$. Taking $n = j+\frac{1}{2}$, the group chain (3.11) becomes

$$\begin{aligned} &\mathbf{Sp}((2j+1)^2) \supset Sp(2j+1) \times O(2j+1), \\ &[(\tfrac{1}{2})^{(2j+1)^2/2}] \qquad\qquad [\mu_1\mu_2\cdots\mu_{j+(1/2)}][\mu_1\mu_2\cdots\mu_{j+(1/2)}], \\ &[(\tfrac{1}{2})^{[(2j+1)^2/2]-1}\tfrac{3}{2}] \end{aligned} \tag{3.15}$$

where we show under each group the IR to which it corresponds.

The proof of the complementarity is delayed until Sec. 5. In the next section we proceed to show a few properties of the IR of the symplectic group and derive a useful expression of its Casimir operator, which we are going to need afterwards.

4. IRREDUCIBLE REPRESENTATIONS AND CASIMIR OPERATOR OF THE UNITARY SYMPLECTIC GROUP

The hwp $\mathbf{P}$ of an IR $[\mu_1\mu_2\cdots\mu_{j+(1/2)}]$ of the group $Sp(2j+1)$ satisfies the system of equations

$$\Lambda_{mm}\mathbf{P} = \mu_{j-m+1}\mathbf{P}, \qquad m>0, \tag{4.1a}$$

$$\Lambda_{mm'}\mathbf{P} = 0, \qquad m>m' \geq -m. \tag{4.1b}$$

It is straightforward to show the well-known property, according to which $[\mu_1\mu_2\cdots\mu_{j+(1/2)}]$ is a partition, i.e., $\mu_1,\mu_2,\ldots,\mu_{j+(1/2)}$ are integers and

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_{j+(1/2)} \geq 0. \tag{4.2}$$

First of all, from (3.2) the operators Λ_{mm} of Eq. (4.1a) are given by

$$\Lambda_{mm} = \mathcal{C}_{mm} - \mathcal{C}_{-m,-m}. \tag{4.3}$$

When applied to $\mathbf{P}$, the operators $\mathcal{C}_{mm}$ and $\mathcal{C}_{-m,-m}$ measure its degree in the creation operators η_{ms}, $s=1,\ldots,n$, and η_{-ms}, $s=1,\ldots,n$, respectively. Thus their eigenvalues are positive or zero integers, so that those of Λ_{mm} are integers too.

We apply now the lowering generators (3.5c) of $Sp(2j+1)$ to $\mathbf{P}$ and calculate the norm of the resulting polynomial. We have

$$\langle 0|(\Lambda_{m'm}\mathbf{P})^+(\Lambda_{m'm}\mathbf{P})|0\rangle \geq 0, \qquad m>m' \geq -m, \tag{4.4}$$

where $|0\rangle$ is the vacuum state of the boson operators. Transforming the inequalities (4.4) with the help of Eqs. (3.3) and (4.1b), we get the relations

$$\langle 0|\mathbf{P}^+[\Lambda_{mm'},\Lambda_{m'm}]\mathbf{P}|0\rangle \geq 0, \qquad m>m' \geq -m. \tag{4.5}$$

From (2.20) and (4.1a), these reduce to

$$\begin{aligned} &\mu_{j-m+1} - \mu_{j-m'+1} \geq 0 \qquad \text{if } m>m'>0, \\ &\mu_{j-m+1} + \mu_{j-|m'|+1} \geq 0 \qquad \text{if } m>0>m'>-m, \\ &4\mu_{j-m+1} \geq 0 \qquad\qquad \text{if } m' = -m, \end{aligned} \tag{4.6}$$

completing thus the proof of (4.2).

The Casimir operator of the symplectic group is given by

$$\Phi = \sum_{mm'} \Lambda_{mm'}\Lambda_{m'm}. \tag{4.7}$$

Its eigenvalue in an IR $[\mu_1\mu_2\cdots\mu_{j+(1/2)}]$ can be found by applying the operator to the hwp of the IR. With the help of the commutation relations (2.20), the expression (4.7) can be transformed into

$$\Phi = 2\sum_{m>0}[\Lambda_{mm}+2m+1]\Lambda_{mm} + 4\sum_{m>0}\times\sum_{m'=-m+1}^{m-1}\Lambda_{m'm}\Lambda_{mm'} + 2\sum_{m>0}\Lambda_{-mm}\Lambda_{m,-m}. \tag{4.8}$$

From Eqs. (4.1), we get

$$\Phi\mathbf{P} = \varphi\mathbf{P}, \tag{4.9}$$

where

$$\varphi = 2\sum_{m>0}^{j+1/2}\mu_{j-m+1}(\mu_{j-m+1}+2m+1), \tag{4.10a}$$

or

$$\varphi = 2\sum_{i=1}\mu_i(\mu_i+2j-2i+3). \tag{4.10b}$$

We are now going to derive an alternative expression for the Casimir operator Φ, in terms of the generators of the group $O(2n)$, which we shall use in the next section. From (3.2), (2.5) and (2.4a), (2.4b), Eq. (4.7) can be transformed into

$$\Phi = 2\Gamma + 2\sum_{mm'}(-1)^{m+m'}\sum_{st}\eta_{ms}\xi_{m's}\eta_{-mt}\xi_{-m't}, \quad (4.11)$$

where

$$\Gamma = \sum_{mm'} \mathcal{C}_{mm'}\mathcal{C}_{m'm} \quad (4.12)$$

is the Casimir operator of the group $\mathfrak{U}(2j+1)$. It is straightforward to show that this operator is connected with the Casimir operator of the subgroup $U(n)$ of $O(2n)$,

$$\Gamma' = \sum_{st} C_{st}C_{ts}, \quad (4.13)$$

by the relation

$$\Gamma = \Gamma' + (2j+1-n)N, \quad (4.14)$$

where

$$N = \sum_{ms}\mathbf{C}_{ms,ms} = \sum_{m}\mathcal{C}_{mm} = \sum_{s}C_{ss} \quad (4.15)$$

is the number operator. We substitute now Eq. (4.14) for the first term of Eq. (4.11), and put the second term of this equation in normal form. The result is

$$\Phi = 2\Gamma' + 2(2j+2-n)N - 2\sum_{st}D^{+}_{st}D_{st}. \quad (4.16)$$

The operator Γ' can be further transformed into

$$\Gamma' = \sum_{s}(C_{ss}+n+1-2s)C_{ss} + 2\sum_{s<t}C_{ts}C_{st}, \quad (4.17)$$

so that finally

$$\Phi = 2\sum_{s}(C_{ss}+2j+3-2s)C_{ss} + 4\sum_{s<t}C_{ts}C_{st} - 2\sum_{st}D^{+}_{st}D_{st}. \quad (4.18)$$

At this point, it is worth while to note that the possibility of writing the Casimir operator of $Sp(2j+1)$ in terms of the generators of $O(2n)$ is directly connected to the complementarity of the two groups. More precisely, it is shown in the Appendix that the sum of the Casimir operators of both groups is equal to a constant.

We proceed now to prove the property stated at the end of Sec. 3.

5. BASIS FOR IRREDUCIBLE REPRESENTATIONS OF THE UNITARY SYMPLECTIC GROUP

We want to show that the linearly independent polynomial solutions of Eqs. (3.14) form a basis for an IR of $Sp(2j+1)$ characterized by the partition $[\mu_1\mu_2\cdots\mu_u]$, $u = \min(j+\frac{1}{2}, n)$, and $\mu_{u+1} = \cdots = \mu_n = 0$ if $n > j+\frac{1}{2}$.

As the operators C_{st} and D_{st} are invariant under the transformations of $Sp(2j+1)$, it is clear that the set of all linearly independent polynomial solutions of Eqs. (3.14) form a basis for a representation of $Sp(2j+1)$. Let us assume that this representation is reducible. We can then choose linear combinations of these polynomials so that in the new basis the representation is explicitly reduced. Owing to a well-known theorem of Cartan,[11] each subset of polynomials that is a basis for an IR has a unique term of highest weight. It can be found by solving Eqs. (3.14) and

$$\Lambda_{mm}\mathbf{P} = \mu'_{j-m+1}\mathbf{P}, \quad m > 0, \quad (5.1a)$$

$$\Lambda_{mm'}\mathbf{P} = 0, \quad m > m' \geq -m \quad (5.1b)$$

simultaneously. Our theorem will thus be proved if we show that the polynomial satisfying both Eqs. (3.14) and (5.1) for a given $[\mu_1\cdots\mu_n]$ is unique and corresponds to $\mu'_1 = \mu_1, \ldots, \mu'_{j+(1/2)} = \mu_{j+(1/2)}$ if $n \geq j+\frac{1}{2}$ and $\mu'_1 = \mu_1, \ldots, \mu'_n = \mu_n, \mu'_{n+1} = 0, \ldots, \mu'_{j+(1/2)} = 0$ if $n < j+\frac{1}{2}$. As the proof is quite similar to that used for the corresponding theorem for the orthogonal group,[4] we shall only give the main steps.

From (2.16), the general solution of Eqs. (3.14a) and (3.14b) is given by

$$P = (\Delta^1_j)^{\mu_1-\mu_2}(\Delta^{1\,2}_{j\,j-1})^{\mu_2-\mu_3}\cdots(\Delta^{1\,2\,\cdots\,n}_{j\,j-1\cdots j-n+1})^{\mu_n} \times Z\left(\frac{\Delta^1_m}{\Delta^1_j}, \frac{\Delta^{1\,2}_{j\,m}}{\Delta^{1\,2}_{j\,j-1}}, \ldots, \frac{\Delta^{1\,2\,\cdots\,n}_{j\,j-1\cdots m}}{\Delta^{1\,2\,\cdots\,n}_{j\,j-1\cdots j-n+1}}\right), \quad (5.2)$$

with $\mu_{j+(3/2)} = \cdots = \mu_n = 0$ in the case $n > j+\frac{1}{2}$. We may, therefore, restrict ourselves to the case $n \leq j+\frac{1}{2}$. The arbitrary polynomial Z has now to be chosen so that P satisfies Eqs. (3.14c) and (5.1).

It is straightforward to show that, instead of the ratios appearing in (5.2), Z can be written equally well in terms of

$$\frac{X_{pq}}{\Delta^{1\,2\,\cdots\,p}_{j\,j-1\cdots j-p+1}\Delta^{1\,2\,\cdots\,q}_{j\,j-1\cdots j-q+1}}, \quad q < p = 2, \ldots, n, \quad (5.3a)$$

and

$$\frac{\Delta^{1\,2\,\cdots\,r-1\;r}_{j\,j-1\cdots j-r+2\;m}}{\Delta^{1\,2\,\cdots\,r-1\;r}_{j\,j-1\cdots j-r+2\;j-r+1}}, \quad r = 1, \ldots, n, \quad m = -j+r-1, \ldots, j-r, \quad (5.3b)$$

where the $\frac{1}{2}(n-1)n$ new variables X_{pq} are defined by

$$X_{pq} = \sum_{m}(-1)^{j-m}\Delta^{1\,2\,\cdots\,p-1\;\;p}_{j\,j-1\cdots j-p+2\;\;m}\Delta^{1\,2\,\cdots\,q-1\;\;q}_{j\,j-1\cdots j-q+2\;\;-m}, \quad q < p = 2, \ldots, n. \quad (5.4)$$

With this change, conditions (5.1b) can be easily imposed. By noting that for any X_{pq}

$$\Lambda_{mm'}X_{pq} = 0, \quad m > m' \geq -m, \quad (5.5)$$

the raising generators of $Sp(2j+1)$, when applied to the polynomial (5.2), only act on the ratios (5.3b).

Let us consider first Eqs. (5.1b) with $m = j$. From definition (3.2) and the fact that the index $-j$ only appears in (5.3b) for $r = 1$, the equation corresponding to $m' = -j$ is equivalent to

$$2\mathcal{C}_{j-j}P = 0 \quad (5.6)$$

or

$$\frac{\partial Z}{\partial(\Delta^1_{-j}/\Delta^1_j)} = 0. \quad (5.7)$$

Therefore, Z does not depend on Δ^1_{-j}/Δ^1_j, and $-j$ does not appear in the variables (5.3b). Consequently the equations corresponding to $m' = -j+1, \ldots, j-1$ are equivalent to

$$\mathcal{C}_{jm'}P = 0 \quad (5.8)$$

or

$$\frac{\partial Z}{\partial(\Delta^1_{m'}/\Delta^1_j)} = 0. \quad (5.9)$$

Thus Z does not depend on $\Delta^{1}_{j,-j+1}/\Delta^{1}_{j}, \ldots, \Delta^{1}_{j-1}/\Delta^{1}_{j}$ either, and the ratios with $r = 1$ disappear from the list (5.3b).

Let us consider now Eqs. (5.1b) with $m = j - 1$. As the index $-j+1$ only appears in (5.3b) for $r = 2$, the equation corresponding to $m' = -j+1$ is equivalent to

$$2\mathcal{C}_{j-1,-j+1}P = 0 \tag{5.10}$$

or

$$\frac{\partial Z}{\partial(\Delta^{1\,2}_{j,-j+1}/\Delta^{1\,2}_{j\,j-1})} = 0. \tag{5.11}$$

Therefore, Z does not depend on $\Delta^{1\,2}_{j,-j+1}/\Delta^{1\,2}_{j\,j-1}$, and $-j+1$ does not appear in the variables (5.3b). Consequently the equations corresponding to $m' = -j+2, \ldots, j-2$ are equivalent to

$$\mathcal{C}_{j-1,m'}P = 0 \tag{5.12}$$

or

$$\frac{\partial Z}{\partial(\Delta^{1\,2}_{jm'}/\Delta^{1\,2}_{j\,j-1})} = 0. \tag{5.13}$$

Thus Z does not depend on $\Delta^{1\,2}_{j,-j+2}/\Delta^{1\,2}_{j\,j-1}, \ldots, \Delta^{1\,2}_{j\,j-2}/\Delta^{1\,2}_{j\,j-1}$, and the ratios with $r = 2$ disappear from the list (5.3b).

Going on like this for the other values of m, we arrive finally at the equations corresponding to $m = j-n+1$, which are satisfied if Z does not depend on the ratios (5.3b) with $r = n$. The equations with $m = j-n, \ldots, \frac{1}{2}$, are then automatically satisfied.

The polynomial satisfying Eqs. (3.14a), (3.14b), and (5.1b) is thus given by (5.2) with Z depending only on the variables (5.3a). It can be written as

$$\begin{aligned} P = \sum_{\{k_{pq}\}} \{ & A_{\{k_{pq}\}} X_{21}^{k_{21}} X_{31}^{k_{31}} X_{32}^{k_{32}} \cdots \\ & \times X_{n1}^{k_{n1}} \cdots X_{n\,n-1}^{k_{n\,n-1}} (\Delta^{1}_{j})^{\mu_1-\mu_2-k_{21}-k_{31}-\cdots-k_{n1}} \\ & \times (\Delta^{1\,2}_{j\,j-1})^{\mu_2-\mu_3-k_{21}-k_{32}-\cdots-k_{n2}} \cdots \\ & \times (\Delta^{1\,2\,\cdots\,n}_{j\,j-1\cdots j-n+1})^{\mu_n-k_{n1}-k_{n2}-\cdots-k_{n\,n-1}} \}, \end{aligned} \tag{5.14}$$

where k_{pq} are nonnegative integers and $A_{\{k_{pq}\}}$ are (as yet) arbitrary constants.

Let us now impose conditions (5.1a) on this polynomial.

It is easily seen that

$$\Lambda_{j-s+1,j-s+1}X_{pq} = \epsilon X_{pq}, \quad s = 1, \ldots, j+\tfrac{1}{2}, \tag{5.15}$$

where

$$\begin{aligned} \epsilon &= 2 \quad \text{if} \quad s \leqslant q-1, \\ &= 1 \quad \text{if} \quad q \leqslant s \leqslant p-1, \\ &= 0 \quad \text{if} \quad s \geqslant p, \end{aligned} \tag{5.16}$$

and

$$\Lambda_{j-s+1,j-s+1}\Delta^{1\,2\,\cdots\,p}_{j\,j-1\cdots j-p+1} = \epsilon'\,\Delta^{1\,2\,\cdots\,p}_{j\,j-1\cdots j-p+1}, \quad s = 1, \ldots, j+\tfrac{1}{2}, \tag{5.17}$$

where

$$\begin{aligned} \epsilon' &= 1 \quad \text{if} \quad s \leqslant p, \\ &= 0 \quad \text{if} \quad s > p. \end{aligned} \tag{5.18}$$

Equations (5.1a) are, therefore, equivalent to the set of $j+\frac{1}{2}$ conditions

$$\begin{aligned} \mu'_1 &= \mu_1 - k_{21} - k_{31} - \cdots - k_{n1}, \\ \mu'_2 &= \mu_2 - k_{21} - k_{32} - \cdots - k_{n2}, \\ &\cdots \\ \mu'_n &= \mu_n - k_{n1} - k_{n2} - \cdots - k_{n\,n-1}, \\ \mu'_{n+1} &= 0, \\ &\cdots \\ \mu'_{j+(1/2)} &= 0. \end{aligned} \tag{5.19}$$

As k_{pq} are nonnegative integers, we deduce from (5.19) that

$$\mu_s \geqslant \mu'_s, \quad s = 1, \ldots, n. \tag{5.20}$$

Equations (5.19) also allow us to express n summation indices k_{pq} in terms of the others; but it is not necessary to do it in detail as we are going to show now that all the k_{pq} are zero.

It only remains now to impose conditions (3.14c). They lead to the relation

$$\sum_{ss'} D^{+}_{ss'} D_{ss'} P = 0, \tag{5.21}$$

which, from (4.8) and (4.18), can be rewritten as

$$\begin{aligned} \{ & \sum_{s} (C_{ss} + 2j + 3 - 2s) C_{ss} + 2 \sum_{s<t} C_{ts} C_{st} \\ & - \sum_{m>0} (\Lambda_{mm} + 2m + 1)\Lambda_{mm} - 2 \sum_{m>0} \\ & \sum_{m'=-m+1}^{m-1} \Lambda_{m'm}\Lambda_{mm'} - \sum_{m>0} \Lambda_{-m\,m}\Lambda_{m,-m} \} P = 0. \end{aligned} \tag{5.22}$$

Taking into account that P already satisfies Eqs. (3.14a), (3.14b), and (5.1), we find the condition

$$\sum_{s=1}^{n} (\mu_s - \mu'_s)(\mu_s + \mu'_s + 2j + 3 - 2s) = 0. \tag{5.23}$$

From (4.2) and (5.20), we know that all the terms of this relation are nonnegative. Thus it can be only satisfied if

$$(\mu_s - \mu'_s)(\mu_s + \mu'_s + 2j + 3 - 2s) = 0, \quad s = 1, 2, \ldots, n. \tag{5.24}$$

The second factor is positive definite (as $n \leqslant j + \frac{1}{2}$), consequently Eqs. (5.24) imply that

$$\mu'_s = \mu_s, \quad s = 1, 2, \ldots, n. \tag{5.25}$$

The proof of the theorem stated at the end of Sec. 3 is thus complete.

Finally as Eqs. (5.19) and (5.25) lead to $k_{pq} = 0$ for any p and q, we have also shown that the hwp of the IR of $\mathcal{S}\rho(2j+1)$, characterized by the partition $[\mu_1\mu_2\cdots\mu_n]$ $n \leqslant j + \frac{1}{2}$, is given, apart from a normalization factor, by

$$\begin{aligned} \mathbf{P} = & (\Delta^{1}_{j})^{\mu_1-\mu_2}(\Delta^{1\,2}_{j\,j-1})^{\mu_2-\mu_3} \cdots (\Delta^{1\,2\,\cdots\,n-1}_{j\,j-1\cdots j-n+2})^{\mu_{n-1}-\mu_n} \\ & \times (\Delta^{1\,2\,\cdots\,n}_{j\,j-1\cdots j-n+1})^{\mu_n}. \end{aligned} \tag{5.26}$$

From this, the whole basis of the IR can be found by applying the lowering generators (3.5c) of $Sp(2j+1)$.

APPENDIX: RELATION BETWEEN THE CASIMIR OPERATORS OF THE GROUPS $Sp(2j+1)$ AND $O(2n)$

We want to derive the precise relationship between the Casimir operator Φ of the group $Sp(2j+1)$, defined by (4.7), and that of the group $O(2n)$, defined by

$$\Phi' = \sum_{st} (D^+_{st}D_{st} + D_{st}D^+_{st}) - 2(\sum_s (H_s)^2 + \sum_{s\neq t} C_{st}C_{ts}). \tag{A1}$$

Equation (A1) looks like the expression (4.16) of the operator Φ. In order to be able to compare them, it is necessary to transform the second and third terms of Eq. (A1). We obtain straightforwardly that

$$\Phi' = 2\sum_{st} D^+_{st}D_{st} - 2\sum_s [H_s - (n-1)]H_s - 2\sum_{s\neq t} C_{st}C_{ts}, \tag{A2}$$

and from (3.8a)

$$\Phi' = 2\sum_{st} D^+_{st}D_{st} - 2\Gamma' - 2(2j+2-n)N + n(2j+1)(n-j-\tfrac{3}{2}), \tag{A3}$$

with Γ' and N defined by (4.13) and (4.15), respectively.

Equations (4.16) and (A3) imply that

$$\Phi + \Phi' = n(2j+1)(n-j-\tfrac{3}{2}). \tag{A4}$$

In particular, for $n = j + \frac{1}{2}$, we find that

$$\Phi + \Phi' = -\tfrac{1}{2}(2j+1)^2. \tag{A5}$$

Note that the fact that the sum of the Casimir operators of the groups $Sp(2j+1)$ and $O(2n)$ is equal to a constant is not sufficient to prove the complementarity of the two groups, because it may happen that two IR of one or both groups, characterized by different partitions, correspond to the same eigenvalue of the Casimir operator.

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On the convergence of separable expansions for the t matrix*

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(Received 8 August 1972)

We obtain theorems on the convergence of separable approximations for t matrices which derive from local potentials. We prove that convergence is impossible in the operator norm and the Hilbert-Schmidt norm. This result is universal and independent of the particular method used to construct the separable approximation.

I. INTRODUCTION

This paper studies the convergence of separable expansions for the off-shell two-body t matrix. Numerous authors[1] have constructed different schemes for obtaining specific finite rank approximations for the t matrix and have studied their convergence in differing model problems. The general aim of all these works is to obtain an accurate expansion of the t matrix which will be suitable for solving Faddeev's equations for the three-body scattering problem. Here we study the convergence of separable t matrix expansions in an abstract format and obtain a theorem which states that convergence in the operator norm is impossible. We prove this general result for any t matrix which is derived from a potential that has some local part.

II. THE NONCOMPACTNESS OF THE t MATRIX

In this section we shall prove that a t matrix derived from a local potential is noncompact. It is this noncompact property that makes the convergence of finite-rank approximations difficult. Here the t matrix we examine is the solution of the Lippmann–Schwinger equation

$$t(z) = v - vg_0(z)t(z) \tag{1}$$

for a two-body interaction v, a complex energy variable z, and a resolvent $g_0(z) = (h_0 - z)^{-1}$ expressed in terms of the free Hamiltonian h_0. The nature of the solutions of this equation expressed in momentum space have been studied in detail by Faddeev.[2] The conditions imposed by Faddeev on the local potential in Eq. (1) are that it satisfies a boundedness property A, in momentum space:

$$\text{A:}\quad |v(\mathbf{p}-\mathbf{p}')| \le C/(1 + |\mathbf{p}-\mathbf{p}'|)^{1+\theta},\ \theta > \tfrac{1}{2}, \tag{2a}$$

where C is a constant. The potential is also assumed to satisfy a smoothness property B, defined by the Holder condition,

$$\text{B:}\quad |v(\mathbf{p}-\mathbf{p}') - v(\mathbf{p}+\Delta\mathbf{p}')| \le C|\Delta\mathbf{p}|^{\mu}/(1 + |\mathbf{p}-\mathbf{p}'|)^{1+\theta} \tag{2b}$$

for all $|\Delta\mathbf{p}| < 1, \mu > 0$. When Eq. (1) is written as an integral equation in momentum space, it takes the form

$$t(\mathbf{p},\mathbf{p}';z) = v(\mathbf{p}-\mathbf{p}') - \int \frac{v(\mathbf{p}-\mathbf{p}'')t(\mathbf{p}'',\mathbf{p}';z)d^3\mathbf{p}''}{\mathbf{p}''^2 - z}. \tag{3}$$

The results of Faddeev that we need in this work are that when the conditions A and B are satisfied then Eq. (3) has a unique solution for all z not at the bound-state energies of $h = h_0 + v$. In this case the solution to Eq. (3) satisfies the estimate

$$|t(\mathbf{p},\mathbf{p}';z)| \le C_1/(1 + |\mathbf{p}-\mathbf{p}'|)^{1+\theta}. \tag{4}$$

In what follows we shall analyze $t(z)$ as a linear operator on the Hilbert space $\mathcal{H}$ of square integrable functions in the three-dimensional momentum variables, i.e., the norm of $f \in \mathcal{H}$ is

$$\|f\|_2 = \left(\int |f(\mathbf{p})|^2 d^3\mathbf{p}\right)^{1/2}. \tag{5}$$

We now want to show that $t(z)$ is noncompact in $\mathcal{H}$. This result is the content of the following two propositions.

Proposition 1: Let condition A be satisfied by the potential v and $\mathrm{Im}\, z \neq 0$; then $t(z)$ is noncompact in $\mathcal{H}$.

Proof: We first note that A implies $vg_0(z)$ is compact. In fact $vg_0(z)$ is a Hilbert–Schmidt operator. This follows by direct calculation. The Hilbert–Schmidt operator norm is defined as

$$\|g_0(z)v\|_{\text{H.S.}} = \iint \left|\frac{v(\mathbf{p}-\mathbf{p}')}{\mathbf{p}'^2 - z}\right|^2 d^3\mathbf{p}\, d^3\mathbf{p}' \le \frac{\pi^2}{|\mathrm{Im}\sqrt{z}\,|}\int |v(\mathbf{p})|^2 d^3\mathbf{p}. \tag{6}$$

The last integral on the right exists if $\theta > \frac{1}{2}$. So $g_0(z)v$ is compact.

Now let us demonstrate that $t(z)$ is noncompact. First, we note that the condition that v is local means that v is a multiplication operator when expressed in coordinate space. Thus it is noncompact. Since the Fourier transformation from coordinate space to momentum space is a unitary transformation, v is noncompact in $\mathcal{H}$. Now we suppose $t(z)$ is compact. We know $vg_0(z)$ is compact, and so will be the product $vg_0(z)t(z)$. Equation (1) tells us that v is the sum of two compact operators. Thus v must be compact. This is a contradiction. So we have shown that $t(z)$ is noncompact. This establishes Proposition 1.

We extend the domain of validity of Proposition 1 to include the entire z plane, excepting a small neighborhood around the bound-state poles of $t(z)$. This extension follows at once from the following lemma.

Lemma 1: Let conditions A and B be satisfied; then the difference $t(z_1) - t(z_2)$ is compact for all z_1 and z_2 in the upper (or lower) half z-plane which excludes the discrete spectra of $h_0 + v$.

Proof: This result is easily established by direct

calculation. We use the well-known identity[3] which contains the full off-shell unitarity in the two-body scattering problem, viz.

$$t(z_1) - t(z_2) = (z_2 - z_1)t(z_1)g_0(z_1)g_0(z_2)t(z_2). \tag{7}$$

The right-hand side of Eq. (7) can be proven Hilbert–Schmidt by using the left to obtain a finite bound on the norm:

$$\begin{aligned}\|t(z_1) - t(z_2)\|^2_{\text{H.S.}} &= \iint \left| t(\mathbf{p},\mathbf{p}';z_1) - t(\mathbf{p},\mathbf{p}';z_2)\right|^2 d^3\mathbf{p}d^3\mathbf{p}' \\ &= |z_2 - z_1|^2 \iint \left| \int \frac{t(\mathbf{p},\mathbf{p}'',z_1)t(\mathbf{p}'',\mathbf{p}';z_2)d^3\mathbf{p}''}{(\mathbf{p}''^2 - z_1)(\mathbf{p}''^2 - z_2)} \right|^2 d^3\mathbf{p}d^3\mathbf{p}' \\ &\le |z_2 - z_1|^2 \iint \left[\int \frac{|t(\mathbf{p},\mathbf{p}'';z_1)\|t(\mathbf{p}'',\mathbf{p}';z_2)|\,d^3\mathbf{p}''}{|\mathbf{p}''^2 - z_1\|\mathbf{p}''^2 - z_2|} \right]^2 \\ &\quad \times d^3\mathbf{p}d^3\mathbf{p}'. \end{aligned} \tag{8}$$

For $\text{Im}z \neq 0$ and employing Faddeev's estimate Eq. (4), we can change the order of integration to obtain

$$\|t(z_1) - t(z_2)\|^2_{\text{H.S.}} \le |z_2 - z_1|^2 \times \left| \int \frac{d^3\mathbf{p}''}{|\mathbf{p}''^2 - z_1\|\mathbf{p}''^2 - z_2|} \right|^2 \left| \int \frac{C d^3\mathbf{p}}{(1 + |\mathbf{p}|)^{2+2\theta}} \right|^2,$$

with

$$|z_2 - z_1|^2 \left| \int \frac{d^3\mathbf{p}''}{|\mathbf{p}''^2 - z_1\|\mathbf{p}''^2 - z_2|} \right|^2 = 4\pi^4 |\sqrt{z_2} - \sqrt{z_1}\,|^2,$$

which is valid for z_2 and z_1 in the same half plane, and

$$\left| \int \frac{C}{(1 + |\mathbf{p}|)^{2+2\theta}} d^3\mathbf{p} \right| = C_1 < \infty \quad \text{for} \quad \theta > \tfrac{1}{2}.$$

We have for all $\text{Im}z \neq 0$

$$\|t(z_1) - t(z_2)\|^2_{\text{H.S.}} \le 4\pi^4 C_1^2 |\sqrt{z_2} - \sqrt{z_1}\,|^2. \tag{9}$$

But the bound on the right may be continued on to the real axis. So the lemma is proved.

We can establish the generalization of Proposition 1.

Proposition 2: Let v satisfy conditions A and B then $t(z)$ is noncompact for all z not belonging to the discrete spectra of $h = h_0 + v$.

Proof: This follows trivally from the above lemma and Proposition 1. Let z_1 lie along the upper portion of the cut along the positive real axis in the complex z plane, i.e., $z_1 = s + io$ where s is positive. Let $\text{Im}z_2 > 0$. Now suppose $t(z_1)$ compact. Then

$$t(z_2) = t(z_1) + [t(z_2) - t(z_1)] \tag{10}$$

implies $t(z_2)$ is compact since it is the sum of two compact operators. This contradicts Proposition 1 so $t(z_1)$ must be noncompact.

III. THE CONVERGENCE OF SEPARABLE EXPANSIONS

We now turn to the implications of Proposition 2 for the convergence of finite rank approximations to $t(z)$. All separable approximations take the form

$$\begin{aligned} t(\mathbf{p},\mathbf{p}';z) &\approx t^N(\mathbf{p},\mathbf{p}';z), \\ t^N(\mathbf{p},\mathbf{p}';z) &= \sum_{i=1}^{N}\sum_{j=1}^{N} c_{ij}(z) f_i(\mathbf{p};z) g_j(\mathbf{p}';z), \end{aligned} \tag{11}$$

where f_i and g_j are square integrable and $c_{ij}(z)$ are constants and N is the order of the finite rank approximation $t^N(z)$. We summarize our conclusion in two propositions.

Proposition 3: Let $t^N(z)$ be any finite rank approximation described above; then the Hilbert–Schmidt norm of the difference $t(z) - t^N(z)$ is infinity.

Proof: Assume $\|t(z)\|_{\text{H.S.}} = B < \infty$, for some $t^N(z)$. Thus $t(z) - t^N(z)$ is compact. The operator $t^N(z)$ is finite rank, so $t(z)$ must be compact. This is a contradiction, so we must have

$$\|t(z) - t^N(z)\|_{\text{H.S.}} = \infty \quad \text{for all} \quad t^N(z). \tag{12}$$

A somewhat less demanding norm for convergence than the Hilbert–Schmidt is the operator norm. For any linear operator A on $\mathcal{K}$, this norm is defined by

$$\|A\| = \inf_{f \in \mathcal{K}} (\|Af\|_2 / \|f\|_2). \tag{13}$$

Our last proposition states that convergence in the operator norm is impossible.

Proposition 4: There does not exist any sequence of separable approximations $\{t^N(z); N = 1, \infty\}$ such that

$$\lim_{N\to\infty} \|t(z) - t^N(z)\| = 0. \tag{14}$$

Proof: Assume that Eq. (14) is true for some sequence $\{t^N(z)\}$; then $t(z)$ is the limit in the operator norm of a sequence of compact operators and is therefore compact.[4] This contradicts the noncompactness of $t(z)$, so Eq. (14) cannot be true.

The results we obtain above, of course, do not preclude a weaker type of convergence. For example, it would be possible

$$\|(t(z) - t^N(z))f\|_2 \to 0 \quad \text{as} \quad N \to \infty$$

for a fixed f in $\mathcal{K}$. What our results do provide is a universal upper bound on the type of convergence possible for a separable expansions, regardless of the method which is used to construct the expansion.

In the results stated above we have assumed the potential is a purely local one. However, the only important aspect of the potential our proofs required is that the potential was noncompact. If we add to any noncompact operator a compact operator the sum remains noncompact. Thus our results extend to potential which are a sum of a local part and a compact part, provided that conditions A and B are satisfied. In order to place these results in the proper perspective, the reader should note that in many applications in scattering theory the operator which appears is the combination $g_0(z)t(z)$ rather than $t(z)$. In general the operator $g_0(z)t(z)$ shares the compactness that $g_0(z)v$ possesses.

ACKNOWLEDGMENT

The author would like to thank Professor R. S. Phillips for helpful discussions of the proofs given above.

*Work supported in part by the U. S. Atomic Energy Commission and the City University of New York Faculty Research Award Program.

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[3]See Ref. 2 for the standard proof of this identity.

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Completeness of the wave operators in the repulsive N-body problem

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Completeness of the wave operators is proved for N equal mass quantum mechanical particles interacting by repulsive forces given by pair potentials $V_{ij}(|x_i - x_j|) = O(|x_i - x_j|^{-1-\epsilon})$, $\epsilon > 0$, which also satisfy certain regularity conditions. In a previous paper an incorrect derivation of this result for the two-body problem was given, which we correct and adapt to the N-body situation.

1. INTRODUCTION

The quantum mechanical motion of N equal mass particles which interact by means of pair potentials V_{ij} is described by the unitary group e^{-iHt} acting on $\mathcal{K} = \mathcal{L}^2(\mathbb{R}^{3N})$, where the Hamiltonian operator H is the self-adjoint realization of the differential operator

$$-\Delta + \sum_{1 \le i < j \le N} V_{ij}(x_i - x_j),$$

where $x_k \in \mathbb{R}^3$ is the position of the kth particle. We shall consider only repulsive Kato potentials which are continuously differentiable in $\mathbb{R}^3 - \{0\}$:

$$r\frac{\partial V}{\partial r}(x) = x \cdot \nabla V(x) \le 0, \qquad x \in \mathbb{R}^2 - \{0\}. \tag{1.1}$$

Two such groups $e^{-iH_1 t}$ and $e^{-iH_2 t}$ may be asymptotically related by the wave operators

$$\Omega_\pm(H_2, H_1) = \lim_{t \to \pm\infty} e^{iH_2 t} e^{-iH_1 t}. \tag{1.2}$$

(All operator limits we consider will be in the strong sense.) The wave operators $\Omega_\pm(H, H_0)(H_0 = -\Delta)$ are known to exist if each potential V_{ij} is short range,[1]

$$|V_{ij}(x)| \le c(1 + r)^{-1-\epsilon}, \tag{1.3}$$

but the completeness of $\Omega_\pm(H, H_0)$, which is equivalent to existence of $\Omega_\pm(H_0, H)$ is more difficult to prove. This has been done for $V(x) = 0(r^{-3-\epsilon})$ in a previous article,[2] hereafter referred to as I. Here we shall prove completeness for repulsive radial potentials with the decay rate (1.3), but with some additional regularity conditions on their first and second derivatives.

The two-body problem is equivalent to the problem of one body with an external potential. Here no regularity conditions are necessary[3] for completeness, even without repulsivity, if one uses estimates on H_0, the fact that H is a short-range perturbation of H_0, and a time independent perturbation argument. In I, Theorem 4.1, a direct time-dependent argument for this result was given (in the repulsive case), but the proof is in error because it depends on I, Theorem 3.3, (b), (c), which are incorrectly demonstrated. The same applies to I, Theorem 3.6, (b), (c), but these were never used. (We are indebted to William Faris for pointing out this error.) In Sec. 2, we give a corrected proof for the one-body problem using similar ideas. This motivates our proof in Sec. 3 for the N-body case.

Let H be a self-adjoint operator on a Hilbert space $\mathcal{K}$ and let T be a bounded operator from $\mathcal{K}$ to $\mathcal{K}'$. T is called *H-smooth* if

$$\int_{-\infty}^{\infty} \|Te^{-itH}\varphi\|^2 dt \le C\,\|\varphi\|^2, \qquad \varphi \in \mathcal{K}. \tag{1.4}$$

If $T_j: \mathcal{K} \to \mathcal{K}'$ is H_j-smooth for $j = 1, 2$ then the time integral of $e^{(iH_1 t)} T_1^* T_2 e^{(-iH_2 t)}$ from 0 to ∞ converges strongly.[2,4] Let us call the collection of linear combinations of such products $\mathcal{I}(H_1, H_2)$.

Theorem 1.1:[2] If $H_1 A - AH_2 \in \mathcal{I}(H_1, H_2)$ then $\lim_{t \to \pm\infty} e^{(iH_1 t)} A e^{(iH_2 t)}$ exists.

Thus, if $H - H_0 = V \in \mathcal{I}(H_0, H)$, then $\Omega_\pm(H_0, H)$ exists and the completeness problem is solved. (Take $A = I$.) In the case under consideration it was shown in I that certain operators essentially belong to $\mathcal{I}(H_0, H)$. Among these are multiplication by $f(x_i - x_j)$ if $f = O(r^{-3-\epsilon})$ at ∞ ($\epsilon > 0$), which gives the result cited above. But the only operators shown to be in $\mathcal{I}(H_0, H)$ with $O(r^{-1-\epsilon})$ decay at ∞ were of the form $hH_0 h$,

$$h(x) = (1 + r^2)^{-(1+\epsilon)/4} \tag{1.5}$$

and $(1 + r)^{-1} r\partial V/\partial r$. The latter tends to decay faster than the potential itself, and the former contains differential operators which do not occur in V. However, convergence of the expressions in Theorem 1.1 does follow for certain choices of A, and from this the wave operators can be obtained.

In addition to the fundamental imperative of mathematical scattering theory (prove completeness with the weakest possible decay at infinity), we have an ulterior motive, namely, to demonstrate the relevance of our generalized scattering condition (1.6) below to the standard theory. To deal with long-range potentials where (1.3) fails, we showed[2] the existence of

$$\omega_\pm(A) = \lim_{t \to \pm\infty} e^{iHt} A e^{-iHt}, \tag{1.6}$$

where A is a continuous function of momentum, i.e., the Fourier transform of multiplication by a continuous function approaching zero at infinity. The existence of this limit is a weaker version of completeness since it states that *every* solution $e^{-iHt}\varphi$ of the Schrödinger equation $i\partial\varphi/\partial t = H\varphi$ resembles a solution of $i\partial\varphi/\partial t = H_0\varphi$ (in some weak sense) at large times.[2] In spite of this, no conclusions about completeness of the wave operators have been shown to follow from the existence of $\omega_\pm$ in those cases where both exist, e.g., the N-body repulsive case with $O(r^{-\alpha})$ potentials, $1 < \alpha < 3$.[2] However, in this paper the existence of $\omega_\pm$ seems to play an essential role.

2. THE ONE-BODY PROBLEM

We shall treat the operator $H = H_0 + V(x)$ on $\mathcal{K} = \mathcal{L}^2(\mathbb{R}^n)$, $n \ge 3$, where V is a Kato potential, i.e., $\|V\varphi\| \le a\|H_0\varphi\| + c\|\varphi\|$, $a < 1$, so that H is self-adjoint on the domain of H_0. We also assume V is continuously differentiable on $\mathbb{R}^n - \{0\}$. Throughout this section h will

represent the function on $\mathbb{R}^n$ given by $h(r) = (1+r^2)^{-(1+\epsilon)/4}$, $0 < \epsilon \leq 1$, $r = |x|$ (and the operator multiplication by this function).

Lemma 2.1: Let $H = H_0 + V$, where $V \geq 0$ satisfies the above conditions and the repulsivity condition $r\partial V/\partial r \leq 0$. Then the following operators are H-smooth:

(a) $r^{-1}h(H+1)^{-1}$,

(b) $h\nabla(H+1)^{-1}: \mathcal{K} \to \mathcal{K} \otimes \mathbf{C}^n$,

(c) $\left(-r\frac{\partial V}{\partial r}\right)^{1/2}(1+r^2)^{-1/4}(H+1)^{-1}$.

Proof: H-smoothness of (a) and (c) were proved in Theorem 3.3 of I. For (b) we note that

$$\|h\nabla\varphi\|^2 = \|\nabla h\varphi\|^2 + (h(\Delta h)\varphi, \varphi) \leq \|\nabla h\varphi\|^2 + c\|r^{-1}h\varphi\|^2. \quad (2.1)$$

The first step is a straightforward computation and the second follows from $|\Delta h| \leq c|r^{-1}h|$. H-smoothness of $\nabla \circ h(H+1)^{-1}$ was established in the proof of Theorem 3.3 of I. This, together with (a) and (2.1), gives the desired result.

Remark 2.2: Suppose $T: \mathcal{K} \to \mathcal{K}'$ is H-smooth. If $S: \mathcal{K}' \to \mathcal{K}''$ is bounded, then ST is H-smooth. If $U: \mathcal{K} \to \mathcal{K}$ is bounded and commutes with e^{-itH} for all t, then TU is H-smooth. (The error in I mentioned above was to call a product TU smooth where U does not commute with H.)

Lemma 2.3: If H_1 and H_2 satisfy the conditions imposed on H in Lemma 2.1, then the following operators belong to $\mathcal{I}(H_1, H_2)$:

(a) $(H_1+1)^{-1}fr^{-2}h^2(H_2+1)^{-1}$, f bounded

(b) $(H_1+1)^{-1}H_0fh^2(H_2+1)^{-1}$, f bounded, $|\nabla f| \leq c/r$.

Proof: By Lemma 2.1(a) the expression (a) is a product $T_1^*T_2$ with T_j H_j-smooth. For (b) observe

$$H_0fh^2\varphi = -\nabla\cdot\nabla(fh^2\varphi) = -\nabla\cdot fh^2\nabla\varphi - \nabla\cdot\nabla(fh^2)\varphi = (h\nabla)^*\{(fh\nabla) + (\nabla f)h + 2f(\nabla h)\}\varphi.$$

By Lemma 2.1(b) $h\nabla(H_1+1)^{-1}$ is H_1-smooth and $fh\nabla(H_2+1)^{-1}$ is also H_2-smooth by Remark 2.2. Since $|\nabla f| \leq c/r$, $|\nabla h| \leq r^{-1}h$, and f is bounded, $\{(\nabla f)h + 2f(\nabla h)\}(H_2+1)^{-1}$ is H_2-smooth by Lemma 2.1(a) and Remark 2.2.

Using Lemma 2.3 and Theorem 1.1, it is possible to prove the existence of certain strong limits. The next lemma allows us to relate these to the wave operators. It will also be used in Sec. 3. The proof is straightforward and we omit it.

Lemma 2.4: Let H_1 and H_2 be self-adjoint operators, and A, B bounded operators, all acting on $\mathcal{K}$. Suppose $\lim_{t\to\pm\infty} e^{(iH_2t)}Ae^{(-iH_2t)} = A_\pm$. Then

$$\lim_{t\to\pm\infty} e^{iH_1t}BAe^{-iH_2t} = \lim_{t\to\pm\infty} e^{iH_1t}Be^{-iH_2t}A_\pm$$

(existence of one side implies existence of the other).

If $e^{iH_1t}Ae^{-iH_2t}$ and its adjoint converge as $t \to \pm\infty$, $\lim_{t\to\pm\infty} e^{(iH_1t)}A^*e^{(-iH_1t)} = A_{1\pm}^*$, $\lim_{t\to\pm\infty} e^{(iH_2t)}Ae^{(-iH_2t)} = A_{2\pm}$ and $A_{1\pm}$ has null space $\{0\}$, then $\Omega_\pm(H_2, H_1)$ exists and its range is the orthocomplement of the null space of $A_{2\pm}$.

Theorem 2.5: Let $H = H_0 + V$ on $\mathcal{K} = \mathcal{L}^2(\mathbb{R}^n)$, where V satisfies the conditions of Lemma 2.1, $V = f_1(1+r^2)^{-(1+\epsilon)/2} + f_2r^{-2}(1+r^2)^{-(1+\epsilon)/2}$, f_1 and f_2 are bounded, and $|\nabla f_1| \leq Cr^{-1}$. Then the wave operators $\Omega_\pm(H, H_0)$ exist, and their range is $\mathcal{K}$.

Proof: We shall prove that $e^{(iH_0t)}(H_0+1)^{-2}H_0(H+1)^{-1}e^{-iHt}$ and its adjoint converge as $t \to \pm\infty$. By Theorem 1.1 it is enough to show that $H_0\{(H_0+1)^{-2}H_0(H+1)^{-1}\} - \{(H_0+1)^{-2}H_0(H+1)^{-1}\}H = (H_0+1)^{-2}H_0V(H+1)^{-1} \in \mathcal{I}(H_0, H)$. This follows from Lemma 2.3, using Remark 2.2. The last statement of Lemma 2.4 applies because

$$\lim_{t\to\pm\infty} e^{iH_0t}(H+1)^{-1}H_0(H_0+1)^{-2}e^{-iH_0t} = -\lim_{t\to\pm\infty} e^{iH_0t}(H+1)^{-1}Ve^{-iH_0t}H_0(H_0+1)^{-3} + H_0(H_0+1)^{-3} = H_0(H_0+1)^{-3},$$

which has trivial null space. The last limit is zero because $(H+1)^{-1}V$ is a compact operator and $e^{(-iH_0t)}$ converges weakly to zero as $t \to \pm\infty$.

Thus Lemma 2.4 implies that $\Omega_\pm(H, H_0)$ exists and has range equal to the orthocomplement of the null space of

$$\lim_{t\to\pm\infty} e^{iHt}(H_0+1)^{-2}H_0(H+1)^{-1}e^{-iHt} = H(H+1)^{-3}.$$

This limit is obtained using weak convergence of e^{-iHt} to zero, which is true because H is absolutely continuous (I, Corollary 3.5.). The null space of $H(H+1)^{-3}$ is $\{0\}$ because $H = H_0 + V \geq H_0$.

3. THE N-BODY PROBLEM

In this section, $\mathcal{K} = \mathcal{L}^2(\mathbb{R}^{3N})$, H_0 is still the self-adjoint Laplacian on $\mathcal{K}$ and

$$H = H_0 + V, \; V = \sum_{1\leq i<j\leq N} V_{ij}(|x_i - x_j|) \quad (3.1)$$

and each V_{ij} is continuously differentiable on $\mathbb{R}^3$. Recall that $x_k \in \mathbb{R}^3$ is the position of the kth particle. For repulsive pair potentials, results similar to Lemmas 2.1 and 2.3 will be proved below. Let $P_{ij} = P_i - P_j$, where $P_k = -i\nabla_k$ is the three-dimensional gradient operator with respect to x_k, acting on $\mathcal{K}$. $P_{ij}^2 = P_{ij}\cdot P_{ij}$ will play the role of H_0; similarly $r_{ij} = |x_i - x_j|$ will replace r.

Lemma 3.1: If H is given by (3.1) and V_{ij} satisfies the repulsivity condition (1.1) for each $1 \leq i < j \leq N$, then the following operators are H-smooth:

(a) $r_{ij}^{-1}h(r_{ij})(H+1)^{-1}$,

(b) $h(r_{ij})P_{ij}(H+1)^{-1}: \mathcal{K} \to \mathcal{K} \otimes \mathbb{C}^3$,

(c) $\left(-r_{ij}\frac{\partial V_{ij}}{\partial r_{ij}}\right)^{1/2}(1+r_{ij}^2)^{-1/4}(H+1)^{-1}$.

Proof: The proof is the same as for Lemma 2.1, replacing $-i\nabla$ by P_{ij}, r by r_{ij}, and $h(r)$ by $h(r_{ij})$; and referring to I, Theorem 3.6 instead of 3.3.

Lemma 3.2: If H_1 and H_2 satisfy the conditions imposed on H in Lemma 3.1, then the following operators belong to $\mathcal{I}(H_1, H_2)$,

(a) $(H_1 + 1)^{-1} f(x_i - x_j) r_{ij}^{-2} h(r_{ij})(H_2 + 1)^{-1}$, f bounded

(b) $(H_1 + 1)^{-1} P_{ij}^2 f(x_i - x_j) h^2(r_{ij})(H_2 + 1)^{-1}$, f bounded, $|\nabla f| \leq c/r$.

Proof: This follows from Lemma 3.1 as Lemma 2.3 follows from Lemma 2.1.

Completeness of the wave operators in the N-body situation would follow from $(H_0 + 1)^{-1} \sum_{i<j} V_{ij} (H + 1)^{-1} \epsilon \mathcal{I}(H_0, H)$. But if $V_{ij}(r) = O(r^{-1-\epsilon})$, Lemma 2.2 gives only $(H_0 + 1)^{-1} P_{ij}^2 V_{ij} (H + 1)^{-1} \in \mathcal{I}(H_0, H)$. This was handled in the one-body case by considering $e^{iHt} A e^{-iH_0 t}$, $A = H_0(H_0 + 1)^{-1}$. Here one would need to take for A a *product* of operators, one factor $P_{ij}^2 (P_{ij}^2 + 1)^{-1}$ for each V_{ij}. By Lemma 2.4 this would imply that the range of $\Omega(H, H_0)$ contains the orthocomplement of the null space of the product of all $\omega_\pm (P_{ij}^2 + 1)^{-1}$. Since none of these factors is as simple as $H(H + 1)^{-1}$, this null space is not obviously $\{0\}$ as in the one-body problem.

Instead, we consider, in place of H_0, operators H_α corresponding to a decomposition α of $\{1, \ldots, N\}$ into clusters, where all potentials connecting different clusters are omitted. Write $i \sim j$ if i and j belong to the same cluster, and $i \not\sim j$ if not:

$$H_\alpha = H_0 + \sum_{i<j,\, i \not\sim j} V_{ij}. \tag{3.2}$$

The convergence of $e^{(iH_2 t)} A e^{(-iH_2 t)}$ is needed to apply Lemma 2.4. For Theorem 2.5, where $A = (H_0 + 1)^{-2} H_0 (H + 1)^{-1}$, this followed by relative compactness of V. In the N-body case, the operators A will be more complicated, but always functions of momentum. Thus we can employ a result proved in I, Theorem 5.3.

Lemma 3.3. If $H = H_0 + V$, where V satisfies (3.1) and each V_{ij} satisfies the repulsivity condition (1.1), then the limits (1.6) exist.

Clearly the map $T \to \omega_\pm(T)$ is a homomorphism of the algebra of momentum operators T into operators commuting with e^{iHt} for all t.

In Theorem 2.5, the fact that $e^{iHt}(H_0 + 1)^{-1} e^{-iHt}$ converges to $(H + 1)^{-1}$ was used. We shall need an analogous fact.

Lemma 3.4. If $H = H_0 + \sum V_{ij}$ satisfies the conditions of Lemma 3.1 and $H' = H - \sum_{i,j \in S} V_{ij}$ for some subset S of the pairs $i, j (i < j)$, then

(i) $\lim_{t \to \pm\infty} V_{ij}(H + 1)^{-1} e^{-iHt} = 0$ for any $i < j$

and

(ii) $\lim_{t \to \pm\infty} e^{iHt}(H' + 1)^{-1} e^{-iHt} = (H + 1)^{-1}$.

Proof: In I, Lemma 3.7, (i) is shown. By the resolvent equation

$$\{(H' + 1)^{-1} - (H + 1)^{-1}\} e^{-iHt} = (H' + 1)^{-1} \times \sum_{i,j \in S} V_{ij} (H + 1)^{-1} e^{-iHt},$$

so (ii) follows.

Theorem 3.5: Let $H = H_0 + V$, where V is given by (3.1). Suppose that each pair potential V_{ij} satisfies the repulsivity condition (1.1), the short range condition (1.3), and finally for $0 < \epsilon$,

$$|\nabla V_{ij}(r)| = f_{ij}(r)^2 (1 + r_{ij}^2)^{-1-\epsilon/2},$$

where $|f_{ij}| \leq C$, $|f_{ij}'| \leq C(1 + r)^{-1}$. Then $\Omega_\pm(H, H_0)$ exists and is complete, i.e., its range is $\mathcal{K}$.

Proof: Induction on the number of particles. The assertion for the 2-body problem is implied by Theorem 2.5. Suppose that it is true for the K-body problem for all $2 \leq K < N$. Then $\Omega_\pm(H_\alpha, H_0)$ exists and has range $\mathcal{K}$ for every nontrivial partition α. We shall prove:

Lemma 3.6. If α is a partition of $\{1, \ldots, N\}$ then $\Omega_\pm(H, H_\alpha)$ exists, and its range is the closure of the range of

$$\omega_\pm \left(\prod_{i \not\sim j} [P_{ij}^2 (H_0 + 1)^{-2}] \right).$$

It will follow by the chain rule that $\Omega_\pm(H, H_0)$ exists and its range contains the orthocomplement of the null space of $\omega_\pm(\Pi_{i \not\sim j}[P_{ij}^2 (H_0 + 1)^{-2}])$ for every partition α. It is sufficient to show that no nonzero vector can belong to this subspace. In fact, if $\varphi_\pm \neq 0$ is such a vector, we claim that

$$\left(\omega_\pm \left(\sum_{i<j} P_{ij}^{\,2} (H_0 + 1)^{-2} \right) \varphi_\pm, \varphi_\pm \right) = 0. \tag{3.3}$$

Now

$$(H(H + 1)^{-2} \varphi_\pm, \varphi_\pm) = (\omega_\pm (H_0 (H_0 + 1)^{-2}) \varphi_\pm, \varphi_\pm)$$

by Lemma 3.4. $NH_0 = (\sum P_i)^2 + \sum_{i<j} P_{ij}^{\,2}$, so since $(\sum P_i)^2$ commutes with H, by (3.3) $(\omega_\pm(H_0(H_0 + 1)^{-2})\varphi_\pm, \varphi_\pm) = 1/N((\sum P_i)^2 \omega_\pm((H_0 + 1)^{-2}) \varphi_\pm, \varphi_\pm) < (H_0(H + 1)^{-1}\varphi_\pm, (H + 1)^{-1}\varphi_\pm) \leq (H(H + 1)^{-2} \varphi_+, \varphi_+)$, a contradiction.

Now we must justify (3.3). For some $i \neq j$

$$0 = (\omega_\pm (P_{ij}^2 (H_0 + 1)^{-2}) \varphi_\pm, \varphi_\pm) = \| \omega_\pm (P_{ij} (H_0 + 1)^{-1}) \varphi_\pm \|^2.$$

If E is the set of indices k such that $\omega_\pm(P_{ik}(H_0 + 1)^{-1}) \varphi_\pm = 0$, then for all $k, m \in E$, $\omega_\pm(P_{km}(H_0 + 1)^{-1})\varphi_\pm = 0$, because $P_{km} = P_{im} - P_{ik}$. If E were not equal to $\{1, \ldots, N\}$, we could divide $\{1, \ldots, N\}$ into two clusters: E and its complement E'. For some $k \in E$ and $k' \in E'$, $\omega_\pm(P_{kk'}(H_0 + 1)^{-1})\varphi_\pm = 0$, contradicting the definition of E. Therefore, $\omega_\pm(P_{ij}(H_0 + 1)^{-1})\varphi_\pm = 0$ for all $i < j$ and (3.3) follows:

$$0 = \left\| \omega_\pm \left(\sum_{i<j} P_{ij} (H_0 + 1)^{-1} \right) \varphi_\pm \right\|^2 = \left(\omega_\pm \left(\sum_{i<j} P_{ij}^2 (H_0 + 1)^{-1} \right) \varphi_\pm, \varphi_\pm \right).$$

Thus the proof of the theorem reduces to:

Proof of Lemma 3.6: By Lemmas 2.4 and 3.3, it is enough to show convergence of

$$e^{iH_\alpha t} \prod_{i \not\sim j} [P_{ij}^2 (H_0 + 1)^{-2}] e^{-iHt}$$

and its adjoint, because

$$\lim_{t \to \pm\infty} e^{iH_\alpha t} \prod_{i \not\sim j} [P_{ij}^2 (H_0 + 1)^{-2}] e^{-iH_\alpha t} = \Omega_\pm(H_\alpha, H_0) \Pi_{i \not\sim j} P_{ij}^2 (H_0 + 1)^{-2} \Omega_\pm(H_\alpha, H_0)^*$$

has trivial null space.

The expression $e^{(iH_\alpha t)}\Pi_{i\neq j}[P_{ij}^2(H_0+1)^{-2}]e^{-iHt}$ is a product of factors $e^{(iH_k t)}A_k e^{(-iH_{k+1}t)}$, $k=1,\ldots,M-1$, where $H_1=H_\alpha, H_M=H$, and for $1\le k\le M-1, H_{k+1}-H_k=V_{ij}$, $A_k=P_{ij}^2(H_0+1)^{-2}$ for some $1\neq j$. Therefore it is enough to show that

$$e^{iH_k t}P_{ij}^2(H_0+1)^{-2}e^{-iH_{k+1}t} \tag{3.4}$$

and its adjoint converges for each k. We will not write down the argument for the adjoint since it is the same as that for (3.4) itself. Convergence of (3.4) follows from convergence of

$$e^{iH_k t}(H_k+1)^{-2}P_{ij}^2(H_{k+1}+1)^{-2}e^{-iH_{k+1}t}. \tag{3.5}$$

For the latter implies that $e^{(iH_k t)}(H_k+1)^{-2}P_{ij}^2(H_0+1)^{-2}e^{(-iH_{k+1}t)}$ converges by Lemma 3.4; this gives convergence of $e^{(iH_k t)}(H_k+1)^{-2}e^{(-iH_{k+1}t)}\omega_\pm(P_{ij}^2(H_0+1)^{-2})$ by Lemmas 2.4 and 3.3; convergence of $e^{(iH_k t)}e^{(-iH_{k+1}t)}\omega_\pm(P_{ij}^2(H_0+1)^{-2})(H_{k+1}+1)^{-2}$ follows by Lemma 3.4; finally $e^{(iH_k t)}P_{ij}^2(H_0+1)^{-2}e^{(-iH_{k+1}t)}(H_{k+1}+1)^{-2}$ converges by Lemmas 2.4 and 3.3, which gives convergence for (3.4) because $(H_{k+1}+1)^{-2}$ has range $\mathcal{K}$.

To prove that (3.5) has strong limits, it is enough by Theorem 1.1 to show that $\mathcal{I}(H_k,H_{k+1})$ contains

$$(H_k+1)^{-2}[H_kP_{ij}^2-P_{ij}^2H_{k+1}](H_{k+1}+1)^{-2}$$
$$=(H_k+1)^{-2}\{[H_k,P_{ij}^2]-P_{ij}^2V_{ij}\}(H_k+1)^{-2}.$$

By Lemma 3.2 (and Remark 2.2) $(H_k+1)^{-2}P_{ij}^2V_{ij}(H_{k+1}+1)^{-2}\in\mathcal{I}(H_k,H_{k+1})$, so it remains to consider the other term. (No such term appears in the one-body argument; it is here we need the extra regularity.) The only nonzero contributions to $[H_k,P_{ij}^2]$ come from terms $[V_{\alpha\beta},P_{ij}^2]$ where α or $\beta=i$ or j, but $\alpha,\beta\neq i,j$. In this case

$$[V_{\alpha\beta},P_{ij}]=i\nabla V_{\alpha\beta}=i[(x_\alpha-x_\beta)/r_{\alpha\beta}]f_{\alpha\beta}^2(1+r_{\alpha\beta}^2)^{-1-\epsilon/2}.$$

Write $g^2=(1+r_{\alpha\beta}^2)^{-1-\epsilon/2}, f=f_{\alpha\beta}, v=(x_\alpha-x_\beta)/r_{\alpha\beta}$. Then

$$[V_{\alpha\beta},P_{ij}^2]=P_{ij}\cdot[V_{\alpha\beta},P_{ij}]+[V_{\alpha\beta},P_{ij}]\cdot P_{ij}$$
$$=iP_{ij}\cdot vf^2g^2+if^2g^2v\cdot P_{ij}$$
$$=ifg\{v\cdot P_{ij}+P_{ij}\cdot v\}fg.$$

(The last step results from a fortunate cancellation of commutators.) $T=v\cdot P_{ij}+P_{ij}\cdot v$ is not bounded, but its product with $(H_k+1)^{-1/2}$ is bounded; therefore we write

$$(1/2i)(H_k+1)^{-1}[V_{\alpha\beta},P_{ij}^2]=fg(H_k+1)^{-1}Tfg$$
$$-(H_k+1)^{-1}[H_k,fg](H_k+1)^{-1/2}[(H_k+1)^{-1/2}T]fg.$$

Since $fg=|\partial V_{\alpha\beta}/\partial r|^{1/2}$, it follows from Lemma 3.1(c) and (a) that $fg(H_j+1)^{-1}$ is H_j-smooth ($j=k,k+1$) and $(H_k+1)^{-1}fg(H_k+1)^{-1}Tfg(H_{k+1}+1)^{-2}$ is in $\mathcal{I}(H_k,H_{k+1})$.

We are left with showing the adjoint of $(H_k+1)^{-1}[H_k,fg](H_k+1)^{-1/2}$ is H_k-smooth.

$$i[H_k,fg]=P_{\alpha\beta}\cdot\nabla(fg)+\nabla(fg)\cdot P_{\alpha\beta}.$$

For the first term this result follows by Lemma 3.1(b) because $|\nabla(fg)|\le ch$, and for the second term it is a consequence of Lemma 3.1(a), $|\nabla(fg)|\le|r^{-1}h|$, and boundedness of $P_{\alpha\beta}(H_k+1)^{-1/2}$.

*Research sponsored by the Air Force Office of Scientific Research, Office of Aerospace Research, under AFSOR Grant 70-1866A.

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Motion of a charged lightlike particle in an external field

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We investigate the behavior of a charged photon in an external field, discussing the general theory and working out some examples. The mathematical basis for the equations of motion is a Stueckelberg action principle combined with a treatment which parallels that of Jacobi's principle.

1. INTRODUCTION

In particle mechanics Hamilton's principle gives the equations of the particle coordinates x^i, $i = 1$ to 3, as functions of the time t; Jacobi's principle gives the equations of the particle's trajectory, e.g., two of the x^i as functions of the third. In the mechanics of Stueckelberg[1] the space and time coordinates x^μ, $\mu = 0$ to 3, are expressed as functions of an independent variable λ, and the corresponding space–time curve is the solution to Euler–Lagrange equations of a Stueckelberg action principle. By applying the method of Jacobi it is possible to generate equations of the space–time trajectory of the curve $x^\mu = x^\mu(\lambda)$, where three of the coordinates are expressed as functions of the fourth.[2] In particular, if the history is that of a particle or photon on Minkowski space–time, then the space–time trajectory Lagrangian, with $x^0 = t$ as the independent variable, generates equations of motion of the spatial coordinates which corresponds to the observer's representations of the curve $x^\mu(\lambda)$. In the case of (everywhere) null space–time curves the passage to the equations of the trajectory requires special treatment, namely the introduction of an additional coordinate ω, whose domain is the positive numbers. We wish to exhibit those equations in a few applications for the case of a charged photon[3] in an external field, with the Stueckelberg Lagrangian defined to be[4]

$$L_S\left(x^\mu, \frac{dx^\mu}{d\lambda}\right) = \frac{1}{2}\left(\frac{dx}{d\lambda}\right)^2 + Q\left(\frac{dx}{d\lambda}\right)\cdot A(x), \tag{1.1}$$

and the integration constant,

$$-p_\lambda = \left(\frac{dx^\mu}{d\lambda}\right)\frac{\partial L_S}{\partial(dx^\mu/d\lambda)} - L_S = \frac{1}{2}\left(\frac{dx}{d\lambda}\right)^2, \tag{1.2}$$

to vanish.

The sign function $\epsilon^0 = \epsilon(dx^0/d\lambda) = \pm 1$ is constant along the curves generated by (1.1) for $p_\lambda \geq 0$ if the $x^\mu(\lambda)$ are infinitely differentiable functions. If $\epsilon^0 = +1$ is assigned to photon histories, $\epsilon^0 = -1$ labels the antiphoton histories. ϵ^0 is not constant if $p_\lambda < 0$ because the resulting curves are everywhere spacelike.

In Sec. 2 we review the general properties of the space–time trajectory equations for a charged photon in an external field; in Sec. 3 we work out examples; in Sec. 4 we summarize our results; and in Sec. 5 we offer a concluding remark about charged lightlike particles in general, referring to other work that has appeared. We attach an appendix to the end on the Hamilton–Dirac canonical formalism for the photon.

2. GENERAL THEORY

The observer's Lagrangians corresponding to the photon curves from (1.1) are[2]

$$L(\mathbf{x}, \omega, \dot{\mathbf{x}}, t) = \tfrac{1}{2}\omega(\dot{\mathbf{x}}^2 - 1) + q[\dot{\mathbf{x}}\cdot\mathbf{A}(x,t) - A^\circ(\mathbf{x},t)], \tag{2.1}$$

where $q = \epsilon^0 Q$ is the charge seen on the photon[5] and ω is a *coordinate* which is required to be positive and whose physical significance appears below[6]; the dots denote differentiation by t. The equations of motion of the photon are the Euler–Lagrange equations for the variation condition,

$$\delta A = \delta\int_{t_1}^{t_2} dt\, L(\mathbf{x}, \omega, \dot{\mathbf{x}}, t) = 0, \tag{2.2}$$

the variations being generated by independent fixed endpoint variations of $\mathbf{x}$ and ω, with $\delta\dot{\mathbf{x}} = (d/dt)\delta\mathbf{x}(t)$. These are

$$d(\omega\dot{\mathbf{x}})/dt = q[\mathbf{E}(\mathbf{x},t) + \dot{\mathbf{x}}\times\mathbf{B}(\mathbf{x},t)], \tag{2.3a}$$

$$\dot{\mathbf{x}}^2 - 1 = 0, \tag{2.3b}$$

where

$$\mathbf{E}(\mathbf{x},t) = -\nabla A^\circ(\mathbf{x},t) - \frac{\partial\mathbf{A}(\mathbf{x},t)}{\partial t}, \tag{2.4a}$$

$$\mathbf{B}(\mathbf{x},t) = \nabla\times\mathbf{A}(\mathbf{x},t). \tag{2.4b}$$

We also may write Eqs. (2.3) in the form

$$\omega\ddot{\mathbf{x}} = q[\mathbf{E}_\perp(\mathbf{x},\dot{\mathbf{x}},t) + \dot{\mathbf{x}}\times\mathbf{B}(\mathbf{x},t], \tag{2.5a}$$

$$\dot{\omega} = q\dot{\mathbf{x}}\cdot\mathbf{E}(\mathbf{x},t), \tag{2.5b}$$

in which

$$\mathbf{E}_\perp(\mathbf{x},\dot{\mathbf{x}},t) \equiv \mathbf{E}(\mathbf{x},t) - \dot{\mathbf{x}}[\dot{\mathbf{x}}\cdot\mathbf{E}(\mathbf{x},t)]. \tag{2.6}$$

For the physical significance of ω we integrate Eq. (2.5b) getting

$$\omega_2 - \omega_1 = q\int_1^2 d\mathbf{x}(t)\cdot\mathbf{E}(\mathbf{x}(t),t), \tag{2.7}$$

which gives the change in ω as the work done on the photon by the field. So ω is the photon's kinetic energy.

We can see the photon theory from another viewpoint and gain further insight by looking at the Hamiltonian formulation. This is complicated by the presence of constraints, which are vanishing functions of the canonical variables, e.g.,

$$p_\omega = \frac{\partial L}{\partial\dot{\omega}} = 0 \tag{2.8}$$

is one. These can be handled by the methods of Hamilton–Dirac theory,[7] and we work this out in the Appendix. The Hamiltonian is

$$H_T = H_T(\mathbf{x}, \mathbf{p}, t) = + \,|\mathbf{p} - q\mathbf{A}(\mathbf{x}, t)| + qA^\circ(\mathbf{x}, t), \quad (2.9)$$

and has no ω, p_ω dependence because the (two) constraints, Eq. (2.8) and

$$\omega - |\mathbf{p} - q\mathbf{A}(\mathbf{x}, t)| = 0, \quad (2.10)$$

have been used to eliminate this pair. The elimination may be understood in the sense that the phase space is "reduced in size", points being identified by only six coordinates instead of eight. Equations (2.8) and (2.9) are regarded as definitions of p_ω and ω. An additional restriction on the space is that the entire surface

$$\Sigma(t): |\mathbf{p} - q\mathbf{A}(\mathbf{x}, t)| = 0 \quad (2.11)$$

has been removed, i.e., for no point $(\mathbf{x}, \mathbf{p})$ is Eq. (2.11) satisfied. So in fact there is an infinite set of phase spaces, one for each value of the time t. This feature guarantees the physical features embodied in the condition $\omega > 0$.

Equations (2.10) and (2.14) below give ω as the magnitude of the photon's momentum, which, therefore, is the same as its kinetic energy by Eq. (2.7). The canonical equations are

$$\dot{\mathbf{x}} = \frac{\partial H_T}{\partial \mathbf{p}} = (\mathbf{p} - q\mathbf{A})\,|\mathbf{p} - q\mathbf{A}|^{-1}, \quad (2.12)$$

$$\dot{\mathbf{p}} = -\frac{\partial H_T}{\partial \mathbf{x}} = -q\nabla A^\circ + q[(\mathbf{p} - q\mathbf{A})\cdot\nabla\mathbf{A} + (\mathbf{p} - q\mathbf{A}) \times (\nabla \times \mathbf{A})]\,|\mathbf{p} - q\mathbf{A}|^{-1}, \quad (2.13)$$

whence

$$\frac{d}{dt}(\mathbf{p} - q\mathbf{A}) = q(\mathbf{E} + \dot{\mathbf{x}} \times \mathbf{B}). \quad (2.14)$$

Equations (2.12) and (2.14) agree with Eqs. (2.3) when account is taken of Eq. (2.10).

The present methods also give the usual equations for particles, the mass $m > 0$ being identified with $+ (2p_\lambda)^{1/2}$. The configuration equations for the particle case transform into Eqs. (2.3a) and (2.5b) under the substitution of ω for $m(1 - \dot{\mathbf{x}}^2)^{-1/2}$, suggesting $m \to 0$ and $|\dot{\mathbf{x}}| \to 1$ jointly, with finite ratio. The particle Hamiltonian with m set equal to zero is the same function as H_T, and the condition

$$|\mathbf{p} - q\mathbf{A}| \neq 0, \quad (2.15)$$

required by removal of $\Sigma(t)$ in the photon case, is unnecessary in the particle case because the kinetic term of the Hamiltonian,

$$[(\mathbf{p} - q\mathbf{A})^2 + m^2]^{1/2}, \quad (2.16)$$

cannot vanish. Finally, there are two general noteworthy homologous features of the single particle and single photon theories: (1) $m > 0$ and $\omega > 0$; and (2) $|\dot{\mathbf{x}}| < 1$ and $\omega \neq 0$. The positivity of m and that of ω are conventions, made possible by the constancy of $\epsilon(dx^0/d\lambda)$, which guarantees that the curves given by (1.1) break up into two kinds for specified values of p_λ. In the case of (2), the inequalities reflect the absence of limiting procedures (keeping L_S free of explicit λ-dependence) which could generate cusps in the curve $x^\mu = x^\mu(\lambda)$, e.g., corresponding to the joining from the past of photon and anti-photon, or particle and anti-particle histories.

Next we look at some examples.

3. EXAMPLES

A. Motion in a uniform constant magnetic field

From Eqs. (2.5) with $\mathbf{B} = \mathbf{B}_0 = \text{const}$ and independent of $\mathbf{x}$, and $\mathbf{E} = 0$,

$$\dot{\omega} = 0, \quad (3.1a)$$

$$\frac{d\dot{\mathbf{x}}}{dt} = \left(-\frac{q\mathbf{B}_0}{\omega}\right) \times \dot{\mathbf{x}}, \quad (3.1b)$$

and the path is a helix. The cyclotron frequency is

$$\Omega = |q|B_0/\omega, \quad (3.2a)$$

which can be compared with the case of a charged particle of mass m with energy $E = m(1 - \dot{\mathbf{x}}^2)^{-1/2}$,

$$\Omega(m) = |q|B_0/E. \quad (3.2b)$$

For circular orbits the radius is given by Eq. (2.3b)

$$r = \omega/|q|B_0, \quad (3.3a)$$

while for particles

$$r(m) = |\boldsymbol{\pi}|/|q|B_0, \quad (3.3b)$$

where $\boldsymbol{\pi} = \mathbf{v}E$ is the particle's momentum.

B. Motion in a uniform constant electric field

From Eq. (2.3a) we have

$$\frac{d}{dt}(\omega\dot{\mathbf{x}} - q\mathbf{E}t) = 0, \quad (3.4)$$

$$\omega\dot{\mathbf{x}} = \omega_0\mathbf{v}_0 + q\mathbf{E}t, \quad (3.5)$$

where $\omega_0 = \omega(0)$ and $\mathbf{v}_0 = \dot{\mathbf{x}}(0)$. The simplest case has $\mathbf{E} \| \pm\, \mathbf{v}_0$, for which

$$\dot{\mathbf{x}}(t) = \mathbf{v}_0, \quad (3.6)$$

$$\omega(t) = \omega_0 \pm qEt, \quad (3.7)$$

where $E = |\mathbf{E}|$. Evidently the solution *allows $\omega(t)$ to vanish*, and to see what that means we go back to the Stueckelberg equations for this example.

For the variation condition based on (1.1),

$$\frac{d^2\mathbf{x}}{d\lambda^2} = Q\mathbf{E}\,\frac{dx^0}{d\lambda}, \quad (3.8a)$$

$$\frac{d^2x^0}{d\lambda^2} = Q\mathbf{E}\cdot\frac{d\mathbf{x}}{d\lambda}, \quad (3.8b)$$

which have the solution

$$\frac{d\mathbf{x}}{d\lambda} = \hat{E}[\hat{E}\cdot\mathbf{C}(\cosh QE\lambda - 1) + C^\circ \sinh QE\lambda] + \mathbf{C}, \quad (3.9a)$$

$$\frac{dx^0}{d\lambda} = \hat{E}\cdot\mathbf{C}\sinh QE\lambda + C^\circ \cosh QE\lambda, \quad (3.9b)$$

where $C^\mu = (d/d\lambda)x^\mu(0)$ and $\hat{E} = |\mathbf{E}|^{-1}\mathbf{E}$. For all λ,

$$\left(\frac{dx}{d\lambda}\right)^2 = C^2, \tag{3.10}$$

with $C^2 = 0$ for photons; also

$$(C^0)^{-1}\mathbf{C} = \left(\frac{d}{d\lambda}x^0(0)\right)^{-1}\frac{d}{d\lambda}\mathbf{x}(0) = \mathbf{v}_0, \tag{3.11}$$

which exists since $C^\mu = 0$ is the uninteresting trivial case, $x^\mu(\lambda) = x^\mu(0) = \text{const.}$[8] Using (3.11), we have

$$\frac{dx^0}{d\lambda} = C^0[\hat{E}\cdot\mathbf{v}_0 \sinh QE\lambda + \cosh qE\lambda], \tag{3.12}$$

which has the constant sign of C^0. If $E = \pm\,\mathbf{v}_0$, then

$$\frac{dx^0}{d\lambda} = C^0 \exp(\pm\, QE\lambda), \tag{3.13}$$

and[2]

$$\omega \equiv \left|\frac{dx^0}{d\lambda}\right| = |C^0| \exp(\pm\, QE\lambda), \tag{3.14}$$

which does *not* vanish for *any value of* λ. Choosing $x^0(0) = 0$ and integrating Eq. (3.9b), we have

$$x^0(\lambda) = (QE)^{-1}C^0[\hat{E}\cdot\mathbf{v}_0(\cosh QE\lambda - 1) + \sinh QE\lambda] \tag{3.15}$$

$$= \pm\,(QE)^{-1}C^0[\exp(\pm\, QE\lambda) - 1]. \tag{3.16}$$

As $Q\lambda \to +\infty$, Eq. (3.14) gives $\omega \to 0$ if $E = -\,\mathbf{v}_0$, but $x^0(\lambda) \to (QE)^{-1}C_0$, which is finite, and equal to $(qE)^{-1}\omega_0$. For $q > 0$ this is the time given by Eq. (3.7) for ω to drop to zero.

Thus, while λ ranges over all values, $x^0(\lambda)$ is bounded. The observer's representation of this is that at the time t for which the solution $\omega(t)$ vanishes, the photon disappears (or appears, depending on the signs)! This cannot happen for a particle because of

$$\left|\frac{dx^0}{d\lambda}\right| = m\left[1 + m^{-2}\left(\frac{d\mathbf{x}}{d\lambda}\right)^2\right]^{1/2} \geq m, \tag{3.17}$$

which means the range of x^0 is infinite if that of λ is.

We give the solution for the case of arbitrary initial angle θ_0 between $\mathbf{v}_0$ and $\mathbf{E}$,

$$\omega(t) = [\omega_0^2 + 2\omega_0 qEt\cos\theta_0 + (qEt)^2]^{1/2}, \tag{3.18}$$

with $\dot{\mathbf{x}}(t)$ given by Eq. (3.5). For $0 < \theta_0 < \pi$, $\omega(t)$ cannot vanish, and it tends to infinity with t. Equation (2.5b) gives

$$q\dot{\mathbf{x}}(t)\cdot\mathbf{E} = \dot{\omega}(t) = \omega^{-1}[\omega_0 qE\cos\theta_0 + (qE)^2 t], \tag{3.19}$$

whose magnitude is smaller than that of qE, so the angle θ remains between 0 and π. The component of photon momentum transverse to $\mathbf{E}$ is conserved by Eq. (2.3a), so the transverse velocity

$$\dot{\mathbf{x}}_\perp(t) = \dot{\mathbf{x}}(t) - [\hat{E}\cdot\dot{\mathbf{x}}(t)]\hat{E} \tag{3.20}$$

is given by

$$\dot{\mathbf{x}}_\perp(t) = \{[\omega(t)]/\omega_0\}^{-1}(\mathbf{v}_0), \tag{3.21}$$

and it goes to zero when $t \to \infty$. In the same limit, $\dot{\mathbf{x}}(t) \to \epsilon(q)E$, so a uniform constant electric field is a photon wind (positive or negative, according to the sign of q).

C. Motion in the field of a uniformly moving point charge

We choose space–time coordinates so the source of the field is at rest, and we assume it to be so massive that its rest frame may be treated as inertial. Then, we may take $\mathbf{A} = 0, A^0 = q'r^{-1}$ and get the Lagrangian in plane polar coordinates as

$$L = \tfrac{1}{2}\omega(\dot{r}^2 + r^2\dot{\theta}^2 - 1) - qq'r^{-1}, \tag{3.22}$$

so that the Hamiltonian is

$$H_T = +\,[p_r{}^2 + r^{-2}(p_\theta)^2]^{1/2} + qq'r^{-1}. \tag{3.23}$$

The solution to the Hamilton–Jacobi equation,

$$-\frac{\partial S}{\partial t} = +\left[\left(\frac{\partial S}{\partial r}\right)^2 + r^{-2}\left(\frac{\partial S}{\partial\theta}\right)^2\right]^{1/2} + qq'r^{-1}, \tag{3.24}$$

namely,

$$S = S(r, \theta, t; J, E) = -\,Et + J\theta \pm \int^r [(E - qq'r^{-1})^2 - J^2r^{-2}]^{1/2}dr, \tag{3.25}$$

where E and J are integration constants[9] and the sign in front of the integral is that of p_r, provides all the information about the photon's motion. In particular, we get the orbits from

$$\frac{\partial S}{\partial J} = \text{const.} \tag{3.26}$$

The answer, for $\alpha E \neq 0$, is

$$lr^{-1} = 1 + \eta\cos\beta(\theta - \theta_0), \qquad |\alpha| < 1, \tag{3.27a}$$

$$lr^{-1} = -1 + \eta\cosh\beta(\theta - \theta_0), \qquad |\alpha| > 1, \tag{3.27b}$$

where

$$\alpha = -\,qq'J^{-1}, \tag{3.28a}$$

$$\eta = |\alpha|^{-1}\epsilon(l)\epsilon(1 + \alpha), \tag{3.28b}$$

$$\beta = |1 - \alpha^2|^{1/2}, \tag{3.28c}$$

$$l = \beta^2 J(\alpha E)^{-1}; \tag{3.28d}$$

and if $|\alpha| = 1$, then

$$\bar{l}r^{-1} = -1 + (\theta - \theta_0)^2, \tag{3.27c}$$

with

$$\bar{l} = 2J|E|^{-1}\epsilon(\alpha E). \tag{3.28e}$$

If $\alpha = 0$, then $E = \omega > 0$ and the orbit is a straight line; and if $E = 0$, the answer is

$$r = r_0 \exp[\pm\,\beta(\theta - \theta_0)], \qquad \alpha \geq 1, \tag{3.27d}$$

with the sign in the argument of the exponential that of p_r. There is no solution for the $E = 0$ case if $\alpha < +1$. Finally θ_0 is a "variable constant", certain angular regions being forbidden [for the forms used in (3.27)] for some of the sign combinations for α, $\alpha + 1$, and E.

For the repulsive case, $\alpha < 0$ and the energy E is positive, so that $l < 0$ (also $\bar{l} < 0$) and η has the opposite sign to $1 + \alpha$ (for $\alpha \neq -1$); the orbits are open and unbounded, as in the particle case.[10] The strong attractive case, $\alpha > 1$, exhibits fall to $r = 0$ for both signs of the energy, again the same as the particle case. In the weak attractive case, $0 < \alpha \leq 1$, all the orbits are open and unbounded, except for the $E = 0$ case of $\alpha = 1$, which gives circles. This is quite different from the particle case, where orbits having $E < m$ are bounded open rosettes and, in the $\alpha^2 \ll 1$ regime, precessing ellipses. But the particle boundedness condition, transposed formally to the photon problem by setting $m = 0$, would give $E < 0$ and that cannot be satisfied when $J > -qq'$ since, by Eq. (3.24),

$$\begin{aligned} E &= -\frac{\partial S}{\partial t} \\ &= +\left[\left(\frac{\partial S}{\partial r}\right) + (Jr^{-1})^2\right]^{1/2} + qq'r^{-1} \\ &\geq J(1-\alpha)r^{-1} \geq 0. \end{aligned}$$

The $E = m$ particle case gives unbounded orbits for $\alpha \leq 1$.

There is only one combination of conditions that yield a bound photon orbit not involving fall to the origin, namely, that of total energy $E = 0$ and angular momentum $J = -qq'$ (for which $\alpha = +1$).

D. Motion in the field of an electromagnetic plane wave

Let the direction of the propagation be the positive z axis: the equations of motion admit the solution $\omega = \omega_0 =$ const and $\dot{\mathbf{x}} = \hat{z}$, with $\hat{z}$ a unit vector along the z axis.

We assume the wave is linearly polarized and that the fields are

$$\mathbf{E} = \hat{x}E_0 \cos fu, \tag{3.29a}$$

$$\mathbf{B} = \hat{y}E_0 \cos fu, \tag{3.29b}$$

$$u \equiv t - z, \tag{3.29c}$$

where f is the circular frequency of the wave. The equations of motion are

$$\frac{d}{dt}\omega\dot{x} = qE_0\dot{u}\cos fu, \tag{3.30a}$$

$$\frac{d}{dt}\omega\dot{y} = 0, \tag{3.30b}$$

$$\frac{d}{dt}\omega(1-\dot{u}) = qE_0\dot{x}\cos fu, \tag{3.30c}$$

$$\dot{\omega} = qE_0\dot{x}\cos fu, \tag{3.30d}$$

and

$$2\dot{u} = \dot{x}^2 + \dot{y}^2 + \dot{u}^2. \tag{3.31}$$

Equations (3.30) can be integrated once; they give

$$k\dot{x} = v_{0x} + V_0 \sin fu, \tag{3.32a}$$

$$k\dot{y} = v_{0y}, \tag{3.32b}$$

$$k\dot{u} = \dot{u}_0, \tag{3.32c}$$

$$f^{-1}\dot{k} = \dot{x}V_0 \cos fu, \tag{3.32d}$$

where

$$k = \omega_0^{-1}\omega, \tag{3.33a}$$

$$V_0 = (\omega_0 f)^{-1}qE_0, \tag{3.33b}$$

$$\omega_0 = \omega(0), \tag{3.33c}$$

$$V_{0x} = \dot{x}(0), \tag{3.33d}$$

$$v_{0y} = \dot{y}(0), \tag{3.33e}$$

$$\dot{u}_0 = \dot{u}(0). \tag{3.33f}$$

Adding the squares of (3.32a)–(3.32c) and using Eqs. (3.31) and (3.32c), we find

$$k = 1 + \dot{u}_0^{-1}v_{0x}V_0 \sin fu + (2\dot{u}_0)^{-1}V_0^2 \sin^2 fu, \quad \dot{u}_0 \neq 0, \tag{3.34}$$

which[11] is positive (*and* bounded) and so, by (3.33a), $\omega(t)$ never vanishes. The primary reason for this is Eq. (3.32c). Multiplying Eq. (3.34) by $\dot{u}$, using Eq. (3.32c) again, and integrating, we get a transcendental equation for $u(t)$,

$$fu = (1 + (4\dot{u}_0/V_0^2))^{-1}[(4\dot{u}_0^2/V_0^2)ft + \sin fu \cos fu - 4(v_{0x}/V_0)(1 - \cos fu)], \tag{3.35}$$

where we have chosen $z(0) = 0$. Similarly, with $x(0) = y(0) = 0$, Eqs (3.32a), (3.32b) give

$$x = f^{-1}(V_0/\dot{u}_0)[fu(v_{0x}/V_0) + 1 - \cos fu], \tag{3.36}$$

$$y = f^{-1}(v_{0y}/\dot{u}_0)fu. \tag{3.37}$$

The first term dominates the right side of Eq. (3.35) at large times

$$(ft)^{-1}fu = 1 - \bar{v}_z + O[(ft)^{-1}], \quad t \text{ large}, \tag{3.38}$$

where $\bar{v}_z$ is the z component of the limiting average velocity,

$$\bar{v}_z = \lim_{t\to\infty} t^{-1}z(t) = v_{0z} + \dot{u}_0[1 + (4\dot{u}_0/V_0^2)]^{-1}, \tag{3.39a}$$

in which $v_{0z} \equiv 1 - \dot{u}_0$. Using (3.38) in Eq. (3.36) and (3.37), we get

$$\bar{v}_x = \lim_{t\to\infty} t^{-1}x(t) = \chi v_{0x} \tag{3.39b}$$

$$\bar{v}_y = \lim_{t\to\infty} t^{-1}y(t) = \chi v_{0y}, \tag{3.39c}$$

where χ is a mean "deflection factor"

$$\chi = \dot{u}_0^{-1}(1 - \bar{v}_z) = (4\dot{u}_0/V_0^2)[1 + (4\dot{u}_0/V_0^2)]^{-1}. \tag{3.40}$$

The square of the limiting average velocity is

$$U^2 = \lim_{t\to\infty}[t^{-1}\mathbf{x}(t)]^2 = \bar{v}_x^2 + \bar{v}_y^2 + \bar{v}_z^2 = 1 - 8(\dot{u}_0^2/V_0^2)[1 + (4\dot{u}_0/V_0^2)]^{-2}, \tag{3.41}$$

which is less than one, as we require. $\dot{\mathbf{x}}(t)$ and $\omega(t)$ return regularly to their initial values, at values of t for which $fu(t) = n\pi$, n an integer, i.e., when

$$ft = ft_n = (1 - \bar{v}_z)^{-1}n\pi + 2\gamma_n \dot{u}_0^{-1}(v_{0x}/\dot{u}_0)V_0, \quad (3.42)$$

where $\gamma_n = 0$ for n even and 1 for n odd. Note[12] $\dot{k}(t_n) = (-1)^n \dot{k}(0)$.

To compute the large time average of a quantity $Q(fu)$,

$$\bar{Q} = \lim_{t\to\infty} t^{-1}\int_0^t Q dt, \quad (3.43)$$

we use Eqs. (3.32c) and (3.34) to write

$$t^{-1}\int_0^t Q dt = \dot{u}_0^{-1}(ft)^{-1}\int_0^w dw\ k(w)Q(w), \quad (3.44)$$

where $w = fu$, and then use (3.35), getting

$$\bar{Q} = \chi \lim_{w\to\infty} w^{-1}\int_0^w dw\ k(w)Q(w). \quad (3.45)$$

In this way, for example, $\bar{k}$ is got from Eq. (3.34) as

$$\bar{k} = \chi \lim_{w\to\infty} w^{-1}\int_0^w dw[1 + \dot{u}_0^{-1}v_{0x}V_0 \sin w + (2\dot{u}_0)^{-1}V_0^2 \sin^2 w]^2, \quad (3.46)$$

$$= \chi[1 + (1 + \dot{u}_0^{-1}v_{0x}^2)(V_0^2/2\dot{u}_0) + (3/8)(V_0^2/2\dot{u}_0)^2]. \quad (3.47)$$

Another quantity is the limiting average displacement from $\bar{v}t$; its components,

$$\bar{x}_0 = \overline{x - \bar{v}_x t} = (f\dot{u}_0)^{-1}V_0(1 - \dot{u}_0^{-1}v_{0x}^2\chi), \quad (3.48a)$$

$$\bar{y}_0 = \overline{y - \bar{v}_y t} = -(f\dot{u}_0)^{-1}V_0\dot{u}_0^{-1}v_{0x}v_{0y}\chi, \quad (3.48b)$$

$$\bar{z}_0 = \overline{z - \bar{v}_z t} = (f\dot{u}_0)^{-1}V_0 v_{0x}\chi, \quad (3.48c)$$

do not vanish in general.

Equation (3.37) shows that if the initial velocity is in the xz plane, then $y = 0$ throughout the motion, which we expect since the Lorentz force cannot develop a component in the y direction. If $v_{0x} = 0$, then $\bar{v}_x = 0$ by Eq. (3.39b), while from Eqs. (3.48), $\bar{y}_0 = \bar{z}_0 = 0$, but $\bar{x}_0 \neq 0$. We note from (3.41) that U is independent of the ratio of v_{0y} to v_{0x} if $v_{0x}^2 + v_{0y}^2 = 2\dot{u}_0 - \dot{u}_0^2$ is fixed.

We examine the case where $(2\dot{u}_0/V_0^2)^{1/2} \equiv \epsilon \ll 1$, for which Eq. (3.35) may be replaced by the approximation

$$\sin\psi = (1 + 2\epsilon^2)\psi - a \doteq \psi - a, \quad (3.49)$$

where

$$\psi = 2fu, \quad (3.50a)$$

$$a = 4\dot{u}_0\epsilon^2 ft - \cdots \equiv a_0 - \cdots, \quad (3.50b)$$

the dots representing a correction, of amount[13] $8[v_{0x}/(2\dot{u}_0)^{1/2}] \times (1 - \cos\frac{1}{2}\psi)\epsilon = O(\epsilon)$. Unless $\psi \doteq 2n\pi$, n an integer, du/dt is very small compared to one owing to Eqs. (3.32c) and (3.34). Away from these regions a is approximately linear in t, the ratio of $\dot{a}$ to the linear approximation, $t^{-1}a_0$, being $1 + O(\epsilon)$. As t approaches the values for which $\psi = 2n\pi$, i.e., by Eq. (3.42), where

$$t = t_n = (f\dot{u}_0)^{-1} \cdot \tfrac{1}{2}n\pi\epsilon^{-2} \times [1 + (4\gamma_n/n\pi)(v_{0x}/\sqrt{2\dot{u}_0})\epsilon + 2\epsilon^2], \quad (3.51)$$

the slopes of $(1 + 2\epsilon^2)\psi$ and $\sin\psi$ in Eq. (3.49) become nearly equal and the intersection point moves somewhat more rapidly along the two curves. As a result the photon spends a relatively small fraction of its time in the neighborhood of its initial velocity and energy. To estimate this amount, we expand Eq. (3.49) for small values of $\psi - 2n\pi \equiv \bar{\psi}$,

$$(\tfrac{1}{2}\epsilon^{-1}\bar{\psi})^3 + 3[(-1)^n v_{0x}/\sqrt{2\dot{u}_0}] \cdot (\tfrac{1}{2}\epsilon^{-1}\psi)^2 + 3 \cdot (\tfrac{1}{2}\epsilon^{-1}\bar{\psi}) \doteq 3\epsilon^{-1}\dot{u}_0 f\tau, \quad (3.52)$$

where $\tau = t - t_n$. From Eq. (3.34), k becomes large if $\frac{1}{2}\bar{\psi}$ strays from zero by amounts much in excess of ϵ, which from (3.50b) and (3.52) means times greater than, or of the order of,

$$\delta t = (f\dot{u}_0)^{-1}\epsilon. \quad (3.53)$$

From (3.51), the ratio of "window" to period is of order,

$$\delta t/(t_{n+1} - t_n) = O(\epsilon^3), \quad (3.54)$$

which is small as claimed above. As long as t is away from the "windows", $t_n \pm \delta t$, k is large, $\dot{u}/\dot{u}_0$ is small, $\omega(t)$ slowly varying, and (for both signs of q) $\dot{\mathbf{x}}(t) \doteq \hat{z}$. So the photon is swept up in the wave and makes only relatively brief returns to its initial velocity and energy. But we notice from Eq. (3.53) that $(2\pi)^{-1}f\delta t$ can be many (wave) cycles long if $\dot{u}_0$ is very small.

From Eq. (3.40), when $\epsilon \ll 1$, we have

$$\chi \doteq 4\dot{u}_0 V_0^{-2} = 2\epsilon^2 \ll 1, \quad (3.55)$$

whence $(\bar{v}_x/v_{0x}) \doteq 2\epsilon^2$, $(\bar{v}_y/v_{0y}) \doteq 2\epsilon^2$, and $(1 - \bar{v}_z)/(1 - v_{0z}) \doteq 2\epsilon^2$; also, to order $O(\epsilon^0)$,

$$\bar{k} \doteq \tfrac{3}{8}\dot{u}_0^{-1}V_0^2 \doteq \tfrac{3}{2}\chi^{-1}, \quad (3.56)$$

so the $t \to \infty$ limit of $\omega(t)$ is much greater than the initial value of ω_0. Equations (3.48) give

$$(\bar{z}_0/\bar{x}_0) \doteq 2v_{0x}\epsilon^2, \quad (3.57a)$$

$$(\bar{y}_0/\bar{x}_0) \doteq -2(\dot{u}_0^{-1}v_{0x}v_{0y})\epsilon^2, \quad (3.57b)$$

both of order ϵ^2, since $|\dot{u}_0^{-1}(v_{0x}v_{0y})| < 1$ by Eq. (3.31). Also,

$$|\bar{x}_0| \doteq f^{-1}(|V_0|/\dot{u}_0) = f^{-1}(2\dot{u}_0^{-1})^{1/2}\epsilon^{-1} \geq f^{-1}\epsilon^{-1} \gg f^{-1}, \quad (3.58a)$$

while from Eq. (3.57a),

$$|\bar{z}_0| \doteq f^{-1} \cdot 4\epsilon(v_{0x}^2/2\dot{u}_0)^{1/2} < f^{-1} \cdot 4\epsilon \ll f^{-1}. \quad (3.58b)$$

Thus, while the average of the z-excursions from $\bar{v}_z t$ is small compared to the wavelength, that of the x excursions from $\bar{v}_x t$ is very large. From Eq. (3.57b),

$$|\bar{y}_0| \doteq f^{-1} \cdot |4V_0^{-1}(\dot{u}_0^{-1}v_{0x}v_{0y})| < f^{-1} \cdot 4|V_0|^{-1}, \quad (3.58c)$$

which can be either small or large; in the latter case $\epsilon \ll 1$ means very nearly parallel longitudinal injection, i.e., $\mathbf{v}_0$ very close to $\hat{z}$.

If the wave is circularly polarized, with field given by

$$\mathbf{E} = E_0(\hat{x}\cos fu + \hat{y}\sin fu), \quad (3.59a)$$

$$\mathbf{B} = E_0(-\hat{x}\sin fu + \hat{y}\cos fu), \tag{3.59b}$$

the equations of motion, which along with (3.31) are

$$\frac{d}{dt}\omega\dot{x} = qE_0\dot{u}\cos fu, \tag{3.60a}$$

$$\frac{d}{dt}\omega\dot{y} = qE_0\dot{u}\sin fu, \tag{3.60b}$$

$$\frac{d}{dt}\omega(1-\dot{u}) = qE_0(\dot{x}\cos fu + \dot{y}\sin fu), \tag{3.60c}$$

$$\dot{\omega} = qE_0(\dot{x}\cos fu + \dot{y}\sin fu), \tag{3.60d}$$

may be trated in the same way. The results are also similar: k is positive and bounded for all t; $\bar{v}_x$ and $\bar{v}_y$ are proportional to a deflection factor $\chi = \dot{u}_0^{-1}(1-\bar{v}_z)$, and $U^2 < 1$; $\mathbf{x}(t)$ and $\omega(t)$ return to their initial values at times $t = t_n$ for which fu is an even integer multiple of π, with $ft_n = (1-\bar{v}_z)^{-1}\cdot 2n\pi$, and also $k(t_n) = +k(0)$; if $v_{0x} = 0$, $\bar{y}_0 = \bar{z}_0 = 0$ again holds, but $v_{0y} = 0$ does not result in no y-motion, as is to be expected from Eq. (3.60b); and if $\epsilon \ll 1$, the photon once again is swept up in the wave with $\bar{\mathbf{v}} \doteq \hat{z}$.

There is one interesting special case of motion in a circularly polarized wave, namely that for which $v_{0x} = 0$ and $v_{0y} = -V_0$, which is possible if $|V_0| \leq 1$. Integrating Eqs. (3.60) for this case we find

$$k\dot{x} = -v_{0y}\sin fu, \tag{3.61a}$$

$$k\dot{y} = v_{0y}\cos fu, \tag{3.61b}$$

$$k\dot{u} = \dot{u}_0, \tag{3.61c}$$

$$f^{-1}\dot{k} = 0, \tag{3.61d}$$

so that $k = 1$, $\dot{u} = \dot{u}_0$, and the path is a helix with axis parallel to $v_{0z}\hat{z}$ and centered on $x = \bar{x}_0 = -(f\dot{u}_0)^{-1}\times v_{0y}$, $y = 0$, and having radius $|\bar{x}_0|$. Equations (3.61a) (3.61b) show that the transverse part of the photon's momentum is parallel to $\mathbf{B}$, which leads to $\dot{\mathbf{x}}\cdot\mathbf{E} = 0$, and Eq. (3.61d) expresses the resulting conservation of the photon's kinetic energy. By Eqs. (3.60c), (3.60d) this is responsible for $\dot{z} = v_{0z} = \text{const}$.

4. SUMMARY

Our principal results are these.

(1) The coordinate ω is identified with the photon kinetic energy and the magnitude of its momentum.

(2) Homologous features of particle theory and photon theory are: (a) $m > 0$, and $\omega > 0$; and (b) $|\dot{\mathbf{x}}| < 1$ for particles, and $\omega \neq 0$.

(3) In a uniform constant magnetic field the particle and photon solutions are the same.

(4) A constant uniform electric field is a photon wind, whose direction depends on the sign of q, the photon's charge. After a finite time it destroys the photon if the initial velocity is along the field and the direction of $(-q\mathbf{E})$.

(5) Particle and photon orbits in a static Coulomb field are similar for the repulsive case and for the strong attractive case, $-qq' > J$. For the weak attractive case $-qq' < J$, the condition $\omega > 0$ keeps the total energy $E = \omega + qq'r^{-1}$ positive and all the orbits are unbounded; this corresponds to the particle case having $E > m$. Since $E < 0$ is impossible here, there is no photon analog to the bound particle orbits which result when $E < m$. There is only one combination of conditions giving a bound photon orbit not involving fall to the center: $E = 0$ and $J = -qq'$, which gives a circle; the corresponding particle orbit, with $E = m$, is unbounded.

(6) The force on a charged photon due to an electromagnetic plane wave propagating along the direction of its motion is zero. If the photon's initial velocity has a component in the plane of a monochromatic wave, the motion is more complicated and the energy ω varies with t, though never vanishing; the photon velocity and energy periodically return to their initial values. If $|(1-v_{0z})^{1/2}f\omega_0(qE_0)^{-1}| \ll 1$, where f is the circular frequency of the wave, the photon is swept up in the wave, its average velocity in the limit of $t \to \infty$ being very close to that of the wave, $\bar{\mathbf{v}} \doteq \hat{z}$, for both signs of q. If the wave is circularly polarized the photon motion can be energy conserving if the initial conditions are suitable; in this case the motion is a helix, with the constant value of $\dot{z} \in (-1, 1)$ arbitrary.

5. CONCLUDING REMARKS

The theoretical properties of charged lightlike particles have not received much attention, perhaps owing to the weight of the Maxwell theory of light, and perhaps also to philosophical and cultural historical reasons. Even the simplest problem, of the field produced by an accelerated lightlike charge, appears not to have been solved in the literature. On the other hand, the problem of constructing classes of solutions to the Maxwell equations, which has been studied, has led to interesting results. In older work, some of the interest was in ether theories; H. Bateman, for example, writing in 1915, constructed solutions which were singular at points moving uniformly with the speed of light.[14] The same approach has been employed somewhat more recently by W. B. Bonnor, who has constructed plane fronted solutions to the Maxwell equations, for which the source is a null current of uniformly moving charge.[15] In addition, the same author also has constructed solutions to the coupled, general relativistic, Einstein–Maxwell equations, with the source identified as a dynamically stable null current of uniformly moving (i.e., geodesic) charge.[16] Other papers dealing with the subject of charged lightlike particles are those of Case and Gasiorowicz,[17] Durand,[18] and Dowker and Dowker,[19] all of which are concerned with field theoretical problems relating to spin.

The mathematical basis of the present papers, as we have said (Sec. 1) is rooted in our modification[2] of Stueckelberg's mechanics.[1] The interpretation of the approach is an important theoretical problem for the approach and we have discussed it already in an exploratory way in other papers.[2,20]

APPENDIX: HAMILTON-DIRAC THEORY FOR THE PHOTON

The generalized momenta for the Lagrangian of Eq. (2.1) are

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}} = \omega\dot{\mathbf{x}} + q\mathbf{A}, \tag{A1}$$

$$p_\omega = \frac{\partial L}{\partial \dot{\omega}} = 0, \tag{A2}$$

and the second equation is a primary constraint in the sense of Dirac.[7,21] Equations (A1) and (A2) may be regarded as specifying a surface in the space of the variables $(\mathbf{x}, \dot{\mathbf{x}}, \mathbf{p}, \omega, \dot{\omega}, p_\omega)$. The Hamiltonian is defined by a Legendre transformation,

$$H = \dot{\mathbf{x}} \cdot \mathbf{p} + \dot{\omega} p_\omega - L(\mathbf{x}, \omega, \dot{\mathbf{x}}, t). \tag{A3}$$

The restriction of (A3) to the surface defined by (A1) and (A2) gives the "weak" Hamiltonian

$$H \approx \tfrac{1}{2}\omega + (2\omega)^{-1}(\mathbf{p} - q\mathbf{A})^2 + qA^0, \tag{A4}$$

the wavy equals sign being used to denote "weak equality," that is equality in the surface of (A1)–(A2). In this surface there is no distinction between Eq. (A4) for the Hamiltonian and the following class of Hamiltonians,

$$H_T = H + ap_\omega \approx H \tag{A5}$$

where a is arbitrary. In the surface extended by "infinitesimal relaxation" of Eq. (A2) there is a distinction and a multiplier a must be found which guarantees the time independence of

$$p_\omega \approx 0 \tag{A2'}$$

for time translations generated by H_T. This leads to Dirac's consistency condition

$$\dot{p}_\omega \approx [p_\omega, H_T] \approx 0, \tag{A6}$$

which for the case at hand gives

$$-\frac{\partial H_T}{\partial \omega} \approx -\tfrac{1}{2} + (\mathbf{p} - q\mathbf{A})^2/2\omega^2 \approx 0 \tag{A7}$$

or

$$\omega \approx |\mathbf{p} - q\mathbf{A}|. \tag{A8}$$

Equation (A8) is a secondary constraint because it came from a consistency condition, and also is required to be weakly time independent;

$$[\omega - |\mathbf{p} - q\mathbf{A}|, H_T] \approx a + q\omega^{-1}(\mathbf{p} - q\mathbf{A}) \cdot \nabla A^0 \approx 0. \tag{A9}$$

and a is determined. Thus, the "total Hamiltonian" is

$$H_T = \omega/2 + (\mathbf{p} - q\mathbf{A})^2/2\omega + qA^0 - qp_\omega\omega^{-1}(\mathbf{p} - q\mathbf{A}) \cdot \nabla A^0, \tag{A10}$$

and there are two canonical constraints,

$$\varphi_1 = p_\omega \approx 0, \tag{A11a}$$

$$\varphi_2 = \omega - |\mathbf{p} - q\mathbf{A}| \approx 0. \tag{A11b}$$

As $[\varphi_1, \varphi_2]$ is nonvanishing these constraints are second class and, hence, can be *used* to eliminate the pair of variables (ω, p_ω) by introducing Dirac's modified Poisson bracket, which in the present instance amounts to no more than dropping the term in the sum involving ω and p_ω differentiations. Before doing this we need to perform a surgical operation on the phase space. Owing to Eq. (A11b), the condition $\omega > 0$ renders the points $(\mathbf{x}, \mathbf{p})$ of the surface

$$\Sigma(t): \ |\mathbf{p} - \mathbf{A}(\mathbf{x}, t)| = 0 \tag{A12}$$

inaccessible to the photon at time t. To include the effects of this condition, we redefine the phase space at time t so as to exclude the points of $\Sigma(t)$; this gives a family of spaces characterized by the explicit time dependence in (A12). The requirement that the photon history not leave the space assures that the condition $\omega \neq 0$ will be respected after the (ω, p_ω) coordinate pair has been eliminated.

Equations (A11) now can be substituted into Eq. (A10) as "strong" equations to give

$$H_T = H_T(\mathbf{x}, \mathbf{p}, t) = + \ |\mathbf{p} - q\mathbf{A}| + qA^0. \tag{A13}$$

The canonical formalism of algebraic relations on this reduced phase space (family), with ω and p_ω absent, automatically respects the constraints, Eqs. (A11).

We remark that the family of phase spaces does not depend on the photon's motion; the t dependence comes from explicit, prescribed t dependence of the external fields.

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[1] E. C. G. Stueckelberg, Helv. Phys. Acta **14**, 588 (1941); Helv. Phys. Acta **15**, 23 (1942).

[2] R. G. Cawley, Int. J. Theor. Phys. 3, 483 (1970); Int. J. Theor. Phys. 7, (1972).

[3] We intend the work photon to be understood in a generic sense, of any "particle" whose world line is everywhere null.

[4] The speed of light is 1, and we use the space-favoring metric.

[5] So if the photon has charge q, the antiphoton has charge $-q$; the positivity of ω keeps photon and antiphoton histories from getting tangled up.

[6] The scale of ω depends on that of λ, $(\omega = |dx^0/d\lambda|)$, and is not determined in the theory of single photon motion. Hence also the factor of 1/2 in the kinetic term of L is a convention.

[7] P. A. M. Dirac, *Lectures on Quantum Mechanics* (Belfer Graduate School of Science, Yeshiva, New York, 1964).

[8] $C^0 = 0$, with $\mathbf{C} \neq 0$ violates $C^2 = 0$.

[9] $\omega > 0$ implies $E - qq'r^{-1} > 0$ since $E = -\partial S/\partial t = H$ so E can be zero or negative. But by suitable choice of coordinates we may arrange to have $J \geq 0$, since $J = \partial S/\partial\theta = p_\theta = \omega r^2\dot{\theta}$. We treat only $J > 0$, since the $J = 0$ case is pure radial motion.

[10] R. G. Cawley, J. Math. Phys. **8**, 2092 (1967).

[11] We assume $\dot{u}_0 \neq 0$ for simplicity; if $\dot{u}_0 = 0$, then $\omega(t) = \omega(0)$ and $x(t) = z$ gives the complete solution.

[12] If we characterize the state of motion by the value of $\dot{\omega}$, in addition to ω and $\dot{\mathbf{x}}$, then the corresponding period is $2\pi f^{-1}(1 - \dot{v}_z)^{-1}$.

[13] By Eq. (3.31), $|v_{0x}/(2\dot{u}_0)^{1/2}| < 1$.

[14] H. Bateman, *The Mathematical Analysis of Electrical and Optical Wave-Motion* (Dover, New York, 1955), Chap. VIII (orig. pub., Cambridge U. P., Cambridge, 1915).

[15] W. B. Bonnor, Int. J. Theor. Phys. 2, 373 (1969).

[16] W. B. Bonnor, Int. J. Theor. Phys. 3, 57 (1970).

[17] K. M. Case and S. G. Gasiorowicz, Phys. Rev. **125**, 1055 (1962).

[18] L. Durand, Phys. Rev. **128**, 434 (1962).

[19] J. S. Dowker and Y. P. Dowker, Proc. R. Soc. A **294**, 175 (1966).

[20] R. G. Cawley, Bull. Am. Phys. Soc. **16**, 116 (1971); Int. J. Theor. Phys. 5, 101 (1972).

[21] The terms "primary constraint" and "secondary constraint" are due to P. Bergmann, however; the original paper by Dirac [Can. J. Math. 2, 129 (1950)] did not introduce this classification.

Nth rank tensor representations of $U(n)$ symmetry adapted to subgroups of the symmetric group S_N

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(Received 24 April 1972)

Representations of the symmetric group S_N symmetry adapted to subgroup sequences

$$S_N \nearrow^{\otimes S_{N_j}} \searrow \otimes S_{iN_j} \quad S_N \searrow_{\otimes S_{iN}} \nearrow \otimes S_{iN_j}$$

are considered using double-coset decomposition. The matrix elements of the double-coset representatives are given and their group theoretical properties are discussed. The matrix elements are identified with the recoupling transformations of the unitary group by considering the tensor representations of the latter. The orthogonality and completeness relations of the symmetric group expressed in terms of double-coset representative matrix elements are used to establish general relations that must be satisfied by the coupling coefficients of the unitary group.

I. INTRODUCTION

Because they facilitate the evaluation of matrix products between states symmetry adapted to different (or the same) subgroup chains, the techniques of double-coset decomposition are finding increasing utility in the analysis of nuclear, atomic and molecular problems.[1,2,3] In earlier works with the same problems in mind, Frame[4] has emphasized the important role of double-coset matrices in analyzing the permutation representations of a finite group. The matrices he introduces are shown to provide a complete expansion bases for any matrix that intertwines two inequivalent irreducible permutation representations of the group. In some of the more recent works,[1,3] novel and at times surprising relations have been developed which on analysis find their origin in the intertwining of the symmetric group algebra with the general linear group algebra by tensor representations.[5]

Kramer,[6], and Kramer and Seligman[1] have demonstrated that outer product coupling coefficients associated with the double cosets of the symmetric group can be identified with recoupling transformations in the unitary unimodular groups. In previous works[3] we have introduced similar coefficients from the point of view that they are elements of the matrix of the double-coset representative in irreducible representations of the symmetric group. It is natural then to consider the usual orthogonality and completeness relations as giving nontrivial summation identities for these coupling coefficients. Because our previous work considered only irreducible representations associated with bipartitions and decomposition into identical subgroup sequences, the coupling process did not introduce problems of multiplicities, and we were able to consider the matrices in the usual sense of representation theory. In this paper we extend these notions to the more general case.

In Sec. II double cosets are introduced. By the use of Schur's lemma the matrix element of the double coset representative is shown to possess certain diagonal properties, but in general it is expressed in mixed bases associated with a given irreducible representation of a group. Nevertheless, the important group relations still apply when expressed in the appropriate double coset form. These results are specifically applied to the symmetric group in Sec. III. We adopt the double coset symbolism of Kramer and Seligman which incorporates the important algebraic features in a suggestive notation.

In Sec. IV we consider the representation of the symmetric group realized by the irreducible tensors of the unitary group. Bases with labels that clearly designate the transformation properties under action of both the symmetric group and the unitary group are used. Coupling in this tensor space can be carried out by two complimentary processes: the Clebsch-Gordan series appropriate to coupling the inner product of the unitary group and projection appropriate to coupling the outer product of the symmetric group. The first process leads to the previously noted identification of the double coset representative matrix elements with the recoupling coefficients of the unitary group Eq. (4.4). The previously developed group relations must be satisfied by the recoupling coefficients. The process of projection results in a rather complex relation Eqs. (4.9, 4.10) between these recoupling coefficients and the Clebsch–Gordan coefficients of the unitary group. This relation in one of its more simple (but nontrivial) forms Eq. (4.13) has appeared in previous work,[7,3] but its general formulation apparently is new.

The difficult problem of multiplicity and the specification of parity and phases are considered in the Appendix.

II. DOUBLE COSET DECOMPOSITION

Any finite group G can be decomposed into a union of disjoint double cosets with respect to any two of its subgroups H and K as

$$G = \bigcup_q HqK = \bigcup_q Kq^{-1}H.$$

The matrix element of the double coset representative q in a *mixed* basis symmetry adapted to the subgroup sequences

$$G \nearrow K \to q^{-1}Hq \cap K \equiv {}^qL \quad G \searrow H \to H \cap qKq^{-1} \equiv L_q$$

on the left (lower) and on the right (upper) can be chosen to have special properties which follow from Schur's lemma. The subgroups ${}^qL$ and L_q are isomorphic under the mapping effected by the action of q; i.e.,

$$ql_i = \mathcal{L}_i q \quad \text{for} \quad l_i \in {}^qL, \mathcal{L}_i \in L_q \quad \text{and all } i.$$

If the same matrix block form $\left[{}^{i\lambda_j}_{m}\ {}^{l}_{n}\right]$ is assigned for representing the corresponding elements of the isomorphic groups in *their respective basis*, then Schur's lemma requires the matrix block of q expressed in the mixed basis to be a multiple of the identity. If the subgroup labeling is $(\lambda, \lambda_j, {}_i\lambda_j, m)$ on the right and $(\lambda, {}_i\lambda, {}_i\lambda'_j, m')$ on the left, where the Greek letters correspond to irreducible representations of the respective groups and the Latin letters indicate the remaining specification within the final irreducible representation, then

$$\begin{bmatrix} \lambda & & \underline{q} & \\ {}_i\lambda, & {}_i\lambda'_j, m' & \lambda_j, & {}_i\lambda_j, m' \end{bmatrix} \equiv \delta^{i\lambda_j i\lambda'_j}\delta_{mm'} \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}_q \tag{2.1}$$

where the symbol on the right has been introduce to correspond to the notation adopted later for the symmetric group. One may also regard the matrix element of q as expressing the unitary transformation between q acting on the bases expressed according to the right sequence and the bases expressed according to the left sequence in which case a symbol

$$\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} \equiv ({}_i\lambda \,|\, \lambda\ {}_i\lambda_j | \lambda_j) \tag{2.1'}$$

might be preferred.

To distinguish distinct but equivalent irreducible representations occurring in the decomposition sequences, additional multiplicity labels could be addended to the above notation.

The important relations that follow from the representation theory of finite groups can be expressed in double coset notation. Any average over the group when expressed in double coset form becomes an average over the subgroups coupled by the double coset representatives. The defining relation for the group $(3-j)$ coefficients becomes

$$\begin{aligned} &\begin{pmatrix} \lambda & \lambda' & \lambda'' \\ {}_i\lambda m & {}_i\lambda' m' & {}_i\lambda'' m'' \end{pmatrix}^* \begin{pmatrix} \lambda & \lambda' & \lambda'' \\ \lambda_j n & \lambda'_j n' & \lambda''_j n'' \end{pmatrix} \\ &= \sum_{\substack{q,\ {}_i\lambda_j \\ {}_i\lambda'_j,\ {}_i\lambda''_j}} \frac{hk}{g} \begin{pmatrix} {}^i\lambda & {}_i\lambda' & {}_i\lambda'' \\ m & m' & m'' \end{pmatrix}^* \begin{pmatrix} {}^i\lambda & {}_i\lambda' & {}_i\lambda'' \\ {}_i\lambda_j p & {}_i\lambda'_j p' & {}_i\lambda''_j p'' \end{pmatrix} \\ &\times \begin{pmatrix} \lambda_j & \lambda'_j & \lambda''_j \\ {}_i\lambda_j p & {}_i\lambda'_j p' & {}_i\lambda''_j p'' \end{pmatrix}^* \begin{pmatrix} \lambda_j & \lambda'_j & \lambda''_j \\ n & n' & n'' \end{pmatrix} \\ &\times \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} \begin{bmatrix} \lambda' & \lambda'_j \\ {}_i\lambda' & {}_i\lambda'_j \end{bmatrix} \begin{bmatrix} \lambda'' & \lambda''_j \\ {}_i\lambda'' & {}_i\lambda''_j \end{bmatrix} / d_q. \end{aligned} \tag{2.2}$$

Besides the explicit summations over the ${}_i\lambda_j$ and q we adopt the convention that repeated Roman indices are to be summed (e.g., p, p', and p''). The factor d_q is the order of the intersection group $|{}^qL| = |L_q| \equiv d_q$. The left hand side of (2.2) must be summed over any multiplicity of λ'' occurring in the decomposition of the inner product $\lambda \boxtimes \lambda'$ in G. In the special cases where one or more of the representations are the totally symmetric representations of the corresponding groups, the $(3-j)$ coefficient is trivial and (2.2) can be correspondingly simplified. In particular, for $\lambda'' = \lambda^0$ one has

$$\begin{bmatrix} \lambda^0 & \lambda^0_j \\ {}_i\lambda^0 & {}_i\lambda^0_j \end{bmatrix} = 1$$

and the group orthogonality relation is obtained

$$\delta^{\lambda\lambda'} = \frac{hk}{g} \sum_{i\lambda_j, q} \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} \begin{bmatrix} \lambda' & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} \frac{[\lambda][{}_i\lambda_j]}{[{}_i\lambda][\lambda_j]\, d_q}, \tag{2.3}$$

where $[\lambda]$ is the dimension of the irreducible representation.

A similar decomposition holds for the matrix basis elements of the group algebra

$$\underline{(\lambda \,|\, {}_i\lambda m; \lambda_j n)} = \frac{hk[\lambda]}{g[{}_i\lambda][\lambda_j]} \sum_{i\lambda_j, q} \underline{({}_i\lambda \,|\, m_j; {}_i\lambda_j p)}\ \underline{q}\ \underline{(\lambda_j \,|\, {}_i\lambda_j p; n)} \times \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} / d_q. \tag{2.4}$$

Note that, even though the subgroup sequences may be different, the basic multiplication rule

$$\underline{(\lambda' \,|\, {}_i\lambda' m; \lambda'_j n')}^{\dagger} \underline{(\lambda \,|\, {}_i\lambda m; \lambda_j n)} = \delta^{\lambda\lambda'} \delta^{i\lambda\ i\lambda'} \underline{(\lambda \,|\, \lambda'_j n'; \lambda_j n)} \tag{2.5}$$

still holds.

Relations involving the class character must be treated with caution. Care must be taken to use matrices in the same representation bases, i.e., $H = K$ and $q = q^{-1}$, so that ${}^qL = L_q$. The character can then be calculated as

$$\mathrm{Tr}(q) = \sum_{\substack{i\lambda_j \\ \lambda_j\ i\lambda_j}} \delta^{i\lambda\lambda_i}\, \delta^{i\lambda_j\ j\lambda_i} [{}_i\lambda_j] \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}. \tag{2.6}$$

The orthogonality between class characters (the completeness relation) then imposes another relation on the matrix elements of these double coset representatives.

III. THE SYMMETRIC GROUP

Consider the group S_N of permutations acting on a set of N elements and the sequence of (direct product) subgroups $\otimes\, S_{N_j}$ and $\otimes\, S_{{}_iN_j}$ corresponding to partitioning of the set into m subsets followed by a second partitioning into m' subsets so that

$$S_N \supset \otimes\, S_{N_j} \supset \otimes\, S_{{}_iN_j}, \quad \sum_{i=1}^{m'} {}_iN_j = N_j, \quad \text{and} \quad \sum_{j=1}^{m} N_j = N.$$

Let the Greek label λ designate the irreducible representations of the symmetric group (i.e., λ stands for a

set of partitions or hook lengths), so that the sequence of labels (considered as sets) $\lambda, \lambda_j, {}_i\lambda_j, {}_i m_j$ designates a basis symmetry adapted to the above subgroup sequence. By the Frobenius reciprocity relation the uniqueness of the set of labels is directly related to the uniqueness in decomposing the associated induced outer product. For purposes of continuity, the discussion of this problem is relegated to the Appendix. Some consistent indexing of the multiplicities is assumed in all the relations that follow.

For the double coset decomposition

$$S_N = \bigcup_q \otimes S_{{}_iN}\, q \otimes S_{N_j}, \tag{3.1}$$

Kramer and Seligman[1] following a suggestion of Hackenbroich introduced a double coset symbol

$$\begin{bmatrix} N & N_j \\ {}_iN & {}_iN_j \end{bmatrix}, \quad \begin{cases} i = 1 \ldots m' \\ j = 1 \ldots m \end{cases},$$

which for a given m' by m set of positive integers ${}_iN_j$ [$(m'-1)\,(m-1)$ of which are independent] uniquely specifies a double coset. The action of the double coset representative q on the set N_j is to transfer ${}_iN_j$ elements to the set ${}_iN$. The correspondence is unique because further action on the left or right of q by permutations from the left or right subgroups merely changes the particular elements involved in the transfer but not the numbers ${}_iN_j$. To avoid misunderstanding, the important relations developed in what follows will also be expressed for the case $m = 2 = m'$, for which the double coset symbol can take the form

$$\begin{bmatrix} N & N_1 & N_2 \\ {}_1N & {}_1N_1{}^0 - k & {}_1N_2{}^0 + k \\ {}_2N & {}_2N_1{}^0 + k & {}_2N_2{}^0 - k \end{bmatrix},$$

where the ${}_iN_j^0$ are any set of admissible positive integers (conveniently taken to correspond to $S_{{}_1N} \otimes S_{{}_2N} \cap S_{N_1} \otimes S_{N_2}$) and k takes all integral values (positive and negative) so that all ${}_iN_j \geq 0$. A particular example of the sets involved is given in Table I.

TABLE I. Possible double coset specification for the decomposition $S_7 = \bigcup_q S_5 \otimes S_2 q S_4 \otimes S_3$ with sets (12345) (67) and (1234) (567), respectively.

k	$({}_iN_j)$	possible q	sets ${}_iN_j$
0	$\begin{pmatrix} 4 & 1 \\ 0 & 2 \end{pmatrix}$	ϵ	$\begin{pmatrix} (1234) & (5) \\ 0 & (67) \end{pmatrix}$
1	$\begin{pmatrix} 3 & 2 \\ 1 & 1 \end{pmatrix}$	(17)	$\begin{pmatrix} (234) & (15) \\ (7) & (6) \end{pmatrix}$
2	$\begin{pmatrix} 2 & 3 \\ 2 & 0 \end{pmatrix}$	(17)(26)	$\begin{pmatrix} (34) & (125) \\ (67) & 0 \end{pmatrix}$

The matrix element $\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}$ associated with the double $\begin{bmatrix} N & N_j \\ {}_iN & {}_iN_j \end{bmatrix}$ requires that the irreducible representations must couple by rows and columns via the outer product of the symmetric group.

For $m = m'$ Kramer[6] has introduced equivalent symbols which he calls $9f$ and $6f$ (one of the ${}_iN_j = 0$) symbols. For $m = 2 = m'$ and λ any bipartition irreducible representation there is no multiplicity problem. The identification of these elements with the corresponding recoupling transformations of $SU(2)$ has been discussed elswhere.[3,6]

The group relations of the previous section can be taken over directly with $g = N!$, $h = \Pi_i {}_iN!$, $k = \Pi_j N_j!$, and $d_q = \Pi_{i,j}\, {}_iN_j!$. In addition, all matrix elements may be considered real and possess the symmetry

$$\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} = (-1)^p \begin{bmatrix} \tilde{\lambda} & \tilde{\lambda}_j \\ {}_i\tilde{\lambda} & {}_i\tilde{\lambda}_j \end{bmatrix}, \tag{3.2}$$

where the tilde represents association with respect to the alternating group and p is the parity of the double coset representative as discussed in Appendix B.

To use (2.6) the double coset representative must belong to the self-inverse class of mutually commuting transpositions (class $2^{\sum_{i>j} {}_iN_j}$). Since the choice of the N_j is at our disposal and the permutation class under consideration is specified by one index, we may choose ${}_1N_2 = N_2$, $N_1 = N - N_2$, ${}_1N_1 = N - 2N_2$ and all other $N_j = 0$ so that

$$\chi^{\lambda}_{2^{N_2}} = \sum_{\lambda_1, {}_1\lambda_2, {}_1\lambda_1} [{}_1\lambda_1][\lambda_2] \begin{bmatrix} \lambda & \lambda_1 & \lambda_2 \\ \lambda_1 & {}_1\lambda_1 & \lambda_2 \\ \lambda_2 & \lambda_2 & 0 \end{bmatrix} = (-1)^{N_2}\, \chi^{\tilde{\lambda}}_{2^{N_2}} \tag{3.3}$$

where the sum is over the irreducible representations such that $\lambda \supset \lambda_1 \cdot \lambda_2 \supset {}_1\lambda_1 \cdot \lambda_2 \cdot \lambda_2$. This relation corresponds to a branching law for characters with the representation dimension being the character of the identity class. It is identical with the usual branching relation[8] for the transpose class $N_2 = 1$, in which case it can be written as

$$\chi^{\lambda}_{2} = \sum_{{}_1\lambda_1} [{}_1\lambda_1] \left\{ \sum_{\lambda_1} \begin{bmatrix} \lambda & \lambda_1 & 1 \\ \lambda_1 & {}_1\lambda_1 & 1 \\ 1 & 1 & 0 \end{bmatrix} \right\}. \tag{3.4}$$

The quantity in brackets is a phase ± 1 or 0 given by the following scheme: If the symbol (ij) means a one node removal from the ith partition (row) followed by a one node removal from the jth partition (row) then

$$\begin{bmatrix} \lambda & {}^{(i)}\lambda & 1 \\ {}^{(i)}\lambda & {}^{(ij)}\lambda & 1 \\ 1 & 1 & 0 \end{bmatrix} = -\begin{bmatrix} \lambda & {}^{(j)}\lambda & 1 \\ {}^{(j)}\lambda & {}^{(ji)}\lambda & 1 \\ 1 & 1 & 0 \end{bmatrix}, \quad \begin{bmatrix} \lambda & {}^{(i)}\lambda & 1 \\ {}^{(i)}\lambda & {}^{(ii)}\lambda & 1 \\ 1 & 1 & 0 \end{bmatrix} = 1,$$

$$\text{and} \quad \begin{bmatrix} \lambda & {}^{(i)}\lambda & 1 \\ {}^{(i)}\lambda & {}^{(i,i-1)}\lambda & 1 \\ 1 & 1 & 0 \end{bmatrix} = -1. \tag{3.5}$$

As shown in the next section these relations are verified for bipartition irreducible representations using the $6-j$ coefficients of $SU(2)$. The completeness relation in the symmetric group requires

$$\sum_{\lambda} \chi^{\lambda}_{2^{N_2}} \chi^{\lambda}_{2^{N_2'}} = \delta^{N_2 N_2'} (N - 2N_2)!\, N_2!\, 2^{N_2}. \tag{3.6}$$

The left-hand sum can be conveniently divided into two

sums over associated and self-associated irreducible representations.

IV. TENSOR COUPLING AND THE UNITARY UNIMODULAR GROUPS

The Nth rank tensor space $(n)^N$ of a basic n dimensional vector is invariant under simultaneous action of the symmetric group S_N and the general linear group $GL(n)$. Weyl, in his development of ideas originating with Schur, has shown that the space can be reduced to the Nth rank tensors of permutation type λ corresponding to partitions of N into no more than n parts, and this space $(n)^N_\lambda$ is irreducible under simultaneous action of S_N and $GL(n)$ (although it is reducible under action of either group individually). That one and the same label λ suffices for indicating the irreducible representations of both groups follows from the fact that they form each others commuting algebra. [Technically, we should specify integral representations of $GL(n)$ but these are all the representations of the unitary subgroups which we consider here.] A basis can be chosen so that for $\pi \in S_N$ and $R \in GL(n)$ the action of the elements considered as operators on the basis can be given as

$$\pi R \left\langle \begin{matrix} m \\ N\lambda n \\ M \end{matrix} \right\rangle = R\pi \left\langle \begin{matrix} m \\ N\lambda n \\ M \end{matrix} \right\rangle = \begin{bmatrix} \lambda & \underline{\pi} \\ m' & m \end{bmatrix} \begin{bmatrix} \lambda & \underline{R} \\ M' & M \end{bmatrix} \left\langle \begin{matrix} m' \\ N\lambda n \\ M' \end{matrix} \right\rangle . \tag{4.1}$$

Summation on repeated Latin indices is assumed. The label m specifies the transformation properties under action of the symmetric group and the label M specifies the transformation properties under action of $GL(n)$ or its subgroups. Associated with a given label M is a weight specification of n integers $W_k \geq 0$, $k = 1, \ldots, n$, giving the number of times the kth element of the n-dimensional space is involved in the polynomial so that $\sum_{k=1}^{n} W_k = N$. Although the rank N and the dimension n can be considered as implicitly contained in the representation label λ, they are explicitly designated for clarity. The notation is similar to that used by Biedenharn[9] and co-workers for labeling tensor operators of $SU(n)$ by Gel'fand patterns. Here, however, the upper label designates the symmetric properties of the tensor vector space. A connection between the two schemes can be made as follows. The upper and lower Gel'fand patterns as used by Biedenharn[10] refer to the classification of the homogeneous polynomials of degree p of N vectors in an n-dimensional space under the action of the unitary groups

$U(Nn) \supset u(N) \times U(n) \supset u(N-1) \times U(n-1) \ldots$. Choosing $p = N$ and restricting to the weight space (of the upper pattern referring to $u(N)$)], $W(i)$,[11] one has a carrier space for the permutation group S_N imbedded in $U(N)$. The upper and lower pattern as used here classifies the transformation properties of these polynomials under action of the group

$$S_N \times U(n).$$

As shown by Weyl two additional relations obtain upon restriction to the unitary unimodular subgroup $SU(n)$ of $GL(n)$:

(1) Tensor spaces of rank N and $N + ne$ are equivalent if their partition label $\{{}^i\lambda\}$ and $\{{}^i\lambda + e\}$ are related by adding a constant integer e to all n parts, $i = 1, \cdots, n$, and (2) the Nth rank tensor space contragradient (complex conjugate for the unitary representations considered here) to $\lambda \equiv \{{}^i\lambda\}$ in $SU(n)$ is equivalent to that with inverted signature (Weyl's terminology), i.e., $\{{}^i\lambda^*\} \to \{-({}^{n+1-i})\lambda\}$, which numbers of course, can be made positive by the addition of a constant to all n parts.

Within an irreducible representation of tensors one is still at liberty to independently choose symmetry adaption sequences for both the symmetric group bases labels and the unitary unimodular bases labels. One can alternately couple tensors by means of the Clebsch–Gordan coefficients (decompose the inner product) of $SU(n)$ or by applying projectors (decompose the outer product) of S_N. We exploit these complimentary procedures and the double coset development of the previous section to establish two nontrivial relations. Consider a coupling scheme appropriate to the sequence of tensor products

$$\left\langle \begin{matrix} m \\ N\lambda n \\ M \end{matrix} \right\rangle \to \underset{j}{\pi} \left\langle \begin{matrix} m_j \\ N_j \lambda_j n_j \\ M_j \end{matrix} \right\rangle \to \underset{i,j}{\pi} \left\langle \begin{matrix} {}_i m_j \\ {}_i N_j \, {}_i\lambda_j \, {}_i n_j \\ {}_i M_j \end{matrix} \right\rangle .$$

The dimensions of ${}_i n_j$ of the subspaces is such that their union spans the covering space $U(n)$, but their intersection can be chosen so as to facilitate particular calculations. Knowing the action of a double coset representative on the final tensor product allows the simple scalar contraction

$$\underset{i,j}{\pi} \left\langle \begin{matrix} {}_i m'_j \\ {}_i N_j \, {}_i\lambda'_j \, {}_i n'_j \\ {}_i M'_j \end{matrix} \right\rangle^{\dagger} q \left\langle \begin{matrix} {}_i m_j \\ {}_i N_j \, {}_i\lambda_j \, {}_i n_j \\ {}_i M_j \end{matrix} \right\rangle = \delta^{i\lambda_j \, i\lambda'_j} \delta_{{}_i m_j \, {}_i m'_j} \delta_{{}_i M_j \, {}_i M'_j} \delta_{({}_i n_j)({}_i n'_j)}, \tag{4.2}$$

where the last delta factor indicates the subspaces must be identical and not just of the same dimension. This is implicitly contained in the third delta factor, but for clarity its explicit expression is preferred here. An Nth rank tensor of $SU(n)$ symmetry adapted to the symmetric subgroup $S_N \supset \otimes S_{Nj}$ can be expanded as

$$\left\langle \begin{matrix} \lambda_j m_j \\ N\lambda n \\ M \end{matrix} \right\rangle = \underset{j}{\pi} \left\langle \begin{matrix} m_j \\ N_j \lambda_j n \\ M_j \end{matrix} \right\rangle (\lambda_j M_j | \lambda M)_n, \tag{4.3}$$

where the expansion coefficients are the Clebsch–Gordan coefficients of $SU(n)$. The scalar contraction

$$\left\langle \begin{matrix} {}_i\lambda' & {}_i\lambda'_j & {}_i m'_j \\ N & \lambda' & n \\ & M' & \end{matrix} \right\rangle^{\dagger} q \left\langle \begin{matrix} \lambda_j & {}_i\lambda_j & {}_i m_j \\ N & \lambda & n \\ & M & \end{matrix} \right\rangle$$

can be evaluated directly as

$$\delta^{\lambda\lambda'} \delta^{MM'} \delta^{i\lambda_j \, i\lambda'_j} \delta_{{}_i m_j \, {}_i m'_j} \begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda' & {}_i\lambda_j \end{bmatrix}$$

from our previous development of the double coset representative matrix element for the symmetric group Eq. (2.1). Alternatively, the two tensors can be expanded in a Clebsch–Gordan series giving

$$\pi_{i,j}({}_i\lambda'_j\ {}_iM'_j;\{{}_i\lambda'\ {}_iM'\}|\lambda'M')^*_n({}_i\lambda_j\ {}_iM_j;\{\lambda_jM_j\}|\lambda M)_n \times \left\langle \begin{matrix} & {}_im'_j \\ {}_iN_j & {}_i\lambda'_j\ n \\ & {}_iM'_j \end{matrix} \right\rangle q \left\langle \begin{matrix} & {}_im_j \\ {}_iN_j & {}_i\lambda_j\ n \\ & {}_iM_j \end{matrix} \right\rangle ,$$

which yields upon considering the action of q on the sets N_j

$$\delta^{i\lambda_j\ i\lambda'_j}\delta_{{}_im_j\,{}_im'_j}({}_i\lambda_j\ {}_iM_j;\{{}_i\lambda'\ {}_iM'\}|\lambda'M')^*_n({}_i\lambda_j\ {}_iM_j;\{\lambda_jM_j\}|\lambda M)_n.$$

Equating the two results and dropping the unnecessary primes yields

$$({}_i\lambda_j\ {}_iM_j;\{{}_i\lambda\ {}_iM\}|\lambda'M')^*_n({}_i\lambda_j\ {}_iM_j;\{\lambda_jM_j\}|\lambda M)_n = \delta^{\lambda\lambda'}\delta_{MM'}\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}. \quad (4.4)$$

The left side of Eq. (4.4) is just a recoupling transformation of $SU(n)$, while the right side is simply the usual statement of Schur's lemma and identifies the recoupling transformation with the previously developed double coset matrix element in a mixed basis corresponding to the two subgroup sequences. The intermediate irreducible representation labels ${}_i\lambda, \lambda_j$ and the summed indices ${}_iM, M_j$ are those necessary to indicate a unique coupling scheme. The problem of uniqueness of the state labeling in decomposing the inner product in $SU(n)$ appropriate to the left side of Eq. (4.4) is identical to the labeling problem that arises in the decomposition of the outer product of the symmetric group appropriate to the right side of Eq. (4.4). Additional labels distinguishing multiplicities will have corresponding significance on both sides of this relation. For clarity we illustrate Eq. (4.4) for the case $m = 2 = m'$:

$$\begin{aligned}({}_1\lambda_1\ {}_1M_1;{}_1\lambda_2\ {}_1M_2|{}_1\lambda\ {}_1M)^*_n({}_2\lambda_1\ {}_2M_1;{}_2\lambda_2\ {}_2M_2|\ {}_2\lambda\ {}_2M)^*_n \\ \times({}_1\lambda\ {}_1M;{}_2\lambda\ {}_2M|\lambda'M')^*_n({}_1\lambda_1\ {}_1M_1;{}_2\lambda_1\ {}_2M_1|\lambda_1M_1)^*_n \\ \times({}_1\lambda_2\ {}_1M_2;{}_2\lambda_2\ {}_2M_2|\lambda_2M_2)_n(\lambda_1M_1;\lambda_2M_2|\lambda M)_n \\ = \delta^{\lambda\lambda'}\delta_{MM'}\begin{bmatrix} \lambda & \lambda_1 & \lambda_2 \\ {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_2 \\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_2 \end{bmatrix}. \end{aligned} \quad (4.4')$$

The left-hand side is the recoupling transformation of four irreducible representations which is proportional to the $(9-j)$ coefficient of the group $SU(n)$.

The group relations that hold because the symbol $\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}$ has the significance of a matrix element with respect to the symmetric group can be applied in their entirety to the recoupling transformations of the unitary group. In particular the orthogonality and completeness relations are nontrivial in their content.

For example the character of the class 2^q for bipartition irreducible representations $[N/2+S, N/2-S]$ is given by the coupling coefficients of $SU(2)$ as

$$\chi^S_q = \sum_{S_1,S_2,{}_1S_1}[{}_1S_1][S_2]\begin{bmatrix} S & S_1 & S_2 \\ S_1 & {}_1S_1 & S_2 \\ S_2 & S_2 & 0 \end{bmatrix}$$

$$= \sum_{S_1,S_2,{}_1S_1}(-1)^{2S}[{}_1S_1][S_2](2S_1+1)\begin{Bmatrix} S & S_1 & S_2 \\ {}_1S_1 & S_1 & S_2 \end{Bmatrix}$$

$$= \sum_{{}_1S_1,S_2}(-1)^{2S}[{}_1S_1][S_2]\left\{\sum_K(-1)^{K+2S+2S_2}\right\},$$

$$0 \le K \le 2S_2, |S-{}_1S_1| \le K \le |S+{}_1S_1|, \quad (4.5)$$

where the second equality follows from the identity of the double coset matrix element with the recoupling coefficient. The last equality can be obtained by using expansion and summation identities found in Edmonds[12] (6-2. 11 and 9). Finally, this expression is easily put in the form

$$\chi^S_q = (-1)^q \sum_{{}_1S_1,S_2}\frac{(-1)^{K_{\min}}+(-1)^{K_{\max}}}{2}[{}_1S_1][S_2], \quad (4.6)$$

with $K_{\min} = |S-{}_1S_1|$ and $K_{\max} = 2S_2$ or $S+{}_1S_1$, whichever is lower. This prescription has been verified for all bipartition representations of the symmetric group up to $N = 7$ and is in accord with Eq. (3.5) of the previous section with $q = 1$ $(S_2 = 1/2)$.

Tensor coupling can also be carried out by the action of matrix basis projectors of S_N on an Nth rank tensor product

$$\left\langle \begin{matrix} k \\ N\lambda n \\ \lambda_jM_jn_j \end{matrix} \right\rangle \equiv \frac{(\lambda|k;\lambda_jn_j)}{\mathcal{N}(\lambda,\lambda_jM_jn_j)_j}\pi\left\langle \begin{matrix} m_j \\ N_j\lambda_jn_j \\ M_j \end{matrix} \right\rangle , \quad (4.7)$$

where the script $\mathcal{N}$ indicates a normalizing constant. The projection process can be considered as the induction relation reciprocal to the generalized branching rule for tensor spaces.[13] Just as the identity (4.4) is independent of the dimension n (λ, of course, must be nonvanishing), so here there is no restriction on the subspace dimensions n_j as long as their union spans the n dimensional space. One can evaluate the scalar contraction

$$\left\langle \begin{matrix} k' \\ N\lambda'n \\ {}_i\lambda\ {}_iM\ {}_in \end{matrix} \right\rangle^\dagger \left\langle \begin{matrix} k \\ N\lambda n \\ \lambda_jM_jn_j \end{matrix} \right\rangle = \delta^{kk'}\delta^{\lambda\lambda'}\delta_{WW'}({}_i\lambda\ {}_iM|\lambda W|\lambda_jM_j)$$

$$= \delta^{kk'}\delta^{\lambda\lambda'}\delta_{WW'}\sum_{\substack{{}_iN_j \\ {}_i\lambda_j \\ {}_iM_j}}\pi_{i,j}\frac{[\lambda]\,{}_iN!N_j!\,[{}_i\lambda_j]}{N!\,[{}_i\lambda][\lambda_j]_iN_j!}\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix} \times \frac{({}_i\lambda_j\ {}_iM_j|{}_i\lambda\ {}_iM)^*_{{}_in}({}_i\lambda_j\ {}_iM_j|\lambda_jM_j)_{n_j}}{\mathcal{N}(\lambda,{}_i\lambda\ {}_iM\ {}_in)\mathcal{N}(\lambda,\lambda_jM_jn_j)}. \quad (4.8)$$

The symbol on the left-hand side allows that a unitary transformation in the space of the irreducible representation λ with weight W may be required. The right-hand side follows from Clebsch–Gordan expansions of the subtensors and application of Eqs. (2.4), (2.5), and (4.2). The structure of this relation can be stated compactly by defining the symbol

$$({}_i\lambda\ {}_iM\ {}_in|\lambda|\lambda_j\ M_j\ n_j) \equiv \sum_{\substack{{}_iN_j \\ {}_i\lambda_j \\ {}_iM_j}}\pi_{i,j}\frac{[{}_i\lambda_j]}{{}_iN_j!}\begin{bmatrix} \lambda & \lambda_j \\ {}_i\lambda & {}_i\lambda_j \end{bmatrix}$$

$$\times({}_{i_j}\lambda\ {}_{i_j}M \mid {}_{i_i}\lambda\ {}_{i_i}M)^{*}_{i^n}({}_{t_j}\lambda\ {}_{t_j}M \mid {}_{j_j}\lambda\ {}_{j_j}M)_{n_j} \tag{4.9}$$

and Eq. (4.8) becomes

$$({}_{i}\lambda\ {}_{i}M|\lambda W|\lambda_j M_j) = ({}_{i}\lambda\ {}_{i}M\ {}_{i}n|\lambda|\lambda_j M_j n_j)$$
$$\times[({}_{i}\lambda\ {}_{i}M\ {}_{i}n|\lambda|\ {}_{i}\lambda\ {}_{i}M\ {}_{i}n)(\lambda_j M_j n_j|\lambda|\lambda_j M_j n_j)]^{-1/2}. \tag{4.10}$$

This relation is, of course, an identity if the decomposition sequences are identical, but it is nontrivial if they differ in any element. Special choices of the starting tensors may facilitate the summations of Eq. (4.9). For example, the orthogonality relation may be used to evaluate

$$({}_{i}\lambda\ {}_{i}Mn|\lambda|\lambda_j M_j n) = \pi_{i,j}\frac{N![{}_{i}\lambda][\lambda_j]}{[\lambda]_i N! N_j!}({}_{i}\lambda\ {}_{i}M|\lambda M)^{*}_{n}(\lambda_j M_j|\lambda M)_n. \tag{4.11}$$

The case with $n_j \cap n_k = \delta_{jk} n_j$ and all $n_j = 1$ corresponds to projecting from totally symmetric tensors with ranks specified by weights $W_j = \lambda^0_j$. The summations in Eq. (4.9) reduce to a single term determined by the intersection of the weights associated with ${}_{i}M$ and the weights W_j. Specifying this intersection number by ${}_{i}W_j = {}_{i}\lambda^0_j$ gives

$$({}_{i}\lambda\ {}_{i}M_i n|\lambda|\lambda^0_j\lambda^0_j\,\mathrm{i}) = \pi_{i,j}\frac{({}_{i_j}\lambda^0\ {}_{i_j}\lambda^0 \mid {}_{i_i}\lambda\ {}_{i_i}M)^{*}_{i^n}}{{}_{i}\lambda^0_j!}\begin{bmatrix}\lambda & \lambda^0_j\\ {}_{i}\lambda & {}_{i}\lambda^0_j\end{bmatrix}. \tag{4.12}$$

As an example of the nontrivial relations implied by Eqs. (4.9, 4.10), consider the case $SU(2)$ (the weights are the state labels M) with ${}_1n = {}_2n = 2; n_1 = 1 = n_2$; and ${}_{i}\lambda = {}_{i}\lambda^0$. Equation (4.10) takes the form

$$\left(\begin{matrix}{}_1\lambda_1{}^0 + {}_1\lambda_2{}^0 & {}_2\lambda_1{}^0 + {}_2\lambda_2{}^0\\ ({}_1\lambda_1{}^0, {}_1\lambda_2{}^0) & ({}_2\lambda_1{}^0, {}_2\lambda_2{}^0)\end{matrix}\middle|\begin{matrix}\lambda\\ ({}_1\lambda_1{}^0 + {}_2\lambda_1{}^0, {}_1\lambda_2{}^0 + {}_2\lambda_2{}^0)\end{matrix}\right)_2 = \left\{\frac{[\lambda]({}_1\lambda_1{}^0 + {}_1\lambda_2{}^0)!({}_2\lambda_1{}^0 + {}_2\lambda_2{}^0)!({}_1\lambda_1{}^0 + {}_2\lambda_1{}^0)!({}_1\lambda_2{}^0 + {}_2\lambda_2{}^0)!}{N!\,{}_1\lambda_1{}^0!\,{}_1\lambda_2{}^0!\,{}_2\lambda_1{}^0!\,{}_2\lambda_2{}^0!}\right\}^{1/2}$$
$$\times\begin{bmatrix}\lambda & {}_1\lambda_1{}^0 + {}_2\lambda_1{}^0 & {}_1\lambda_2{}^0 + {}_2\lambda_2{}^0\\ {}_1\lambda_1{}^0 + {}_1\lambda_2{}^0 & {}_1\lambda_1{}^0 & {}_1\lambda_2{}^0\\ {}_2\lambda_1{}^0 + {}_2\lambda_2{}^0 & {}_2\lambda_1{}^0 & {}_2\lambda_2{}^0\end{bmatrix}. \tag{4.13}$$

By using Eq. (4.4a), this expresses any Clebsch–Gordan coefficient of $SU(2)$ in terms of a recoupling transformation of four angular momenta. Kramer and Seligman[7] have used this relation to explain the Regge symmetries of the $(3-j)$ coefficients in $SU(2)$.

V. DISCUSSION

Any problem involving the coupling of identical particles in initially distinct clusters utilizes implicitly or explicitly the double coset representative matrix elements as coupling coefficients. Therefore, such problems utilize recoupling transformations of $SU(n)$ regardless of any spatial significance that this group may or may not have. Thus, the tensor representations of these groups are of interest to physics even apart from any fundamental significance they may have for classifying the internal symmetries of elementary particles. Of course, this has been recognized in atomic theory since the beginning years of quantum mechanics and especially since the works of Racah[14], but attention has mainly been centered on the atomic and nuclear problems because of their spherical symmetry. A principal aspect of so-called spin free quantum chemistry[15] is that the spin multiplicity label retains significance in the evaluation of orbital matrix elements even after all spin integrals have been done. The coupling of multiplicities from different clusters can be effected if the coupling coefficients for the outer product of the symmetric group are known. Because atomic or molecular problems have multiplicities that can be classified with respect to $SU(2)$ for which the Clebsch–Gordan coefficients and the recoupling transformations are tabulated or calculable, the coefficients required for coupling cluster multiplicities are known. Indeed, they provide valuable checks for the relations developed here. For higher dimensional unitary unimodular groups, special choices of the labels in Eq. (4.10) can produce simple closed formulas for certain Clebsch–Gordan coefficients, but the real value of this relation may be in how it compliments the usual algebraic approach.

There are many aspects of the intertwining that seemingly require more study. Aside from the fact that the irreducible representation λ establishes the minimum dimension for which the double coset symbol has meaning, Eqs. (4.4 and 4.10) relate an object of the symmetric group which can depend on N but not on n with an object of the unitary group $U(n)$. On the one hand the double coset matrix element retains this value in higher dimensional unitary spaces, while on the other hand the Weyl equivalence condition relates similar quantities of different tensor rank in $SU(n)$. Also, on the one hand the process of complex conjugation in $SU(n)$ relates in general inequivalent tensor representations of different rank, while on the other hand in the symmetric group S_N the process of association with respect to the alternating group relates, in general, inequivalent tensor representations of the same rank, but in unitary spaces with different dimensions. Finally, the completeness relation as applied to the symmetric group puts additional conditions on the coupling coefficients for tensors of the same rank but of different dimensions.

ACKNOWLEDGMENTS

The author wishes to thank Professor Bruno Gruber for many helpful discussions. In our previous work (Ref. 3) we regret the omission of reference to the works of Kramer and Seligman. Their studies, of course, have been an essential starting point for the work reported here.

APPENDIX A: UNIQUENESS OF THE BASIS LABELS AND THE DOUBLE COSET SYMBOL

Nonuniqueness of the basis labels can result for two different reasons:

1. multiplicities arising from partitions into more than two parts, and
2. multiplicities inherent in decomposing the outer product of two irreducible representations of the symmetric group.

The second reason is the fundamental multiplicity problem in decomposing the inner product of the unitary group. Aside from some structural interpretation nothing new is presented here. The first difficulty can be overcome by introducing intermediate coupling steps so that each step reduces to the fundamental process of coupling binary parts. We consider this first.

Specifying intermediate coupling steps corresponds to a process of contraction[2] of the double coset symbols and simple multiplication of the fundamental matrix elements for subgroup partitions into two parts (the $9f$ elements of Kramer[6]) at each step. It is sufficient to show this for one step say on the right corresponding to the double coset decomposition

$$S_N = \bigcup_q S_{{}_1N\otimes{}_2N}\, q\, S_{N_1\otimes N_2} = \bigcup_{p,q} S_{{}_1N\otimes{}_2N}\, q\, S_{{}_1N_1\otimes{}_1N_2\otimes{}_2N_1\otimes{}_2N_2} \times p S_{N_{1a}\otimes N_{1b}\otimes N_2} = \bigcup_{p,q} S_{{}_1N\otimes{}_2N}\, qp\, S_{N_{1a}\otimes N_{1b}\otimes N_2}.$$

The double coset symbols q and qp are related by the contraction–expansion relation

$$\begin{bmatrix} N & N_1 & N_2 \\ {}_1N & {}_1N_1 & {}_1N_2 \\ {}_2N & {}_2N_1 & {}_2N_2 \end{bmatrix}_q \Longleftrightarrow \begin{bmatrix} N & N_{1a} & N_{1b} & N_2 \\ {}_1N & {}_1N_{1a} & {}_1N_{1b} & {}_1N_2 \\ {}_2N & {}_2N_{1a} & {}_2N_{1b} & {}_2N_2 \end{bmatrix}_{qp}$$

for all integers such that

$$\begin{pmatrix} N_1 \\ {}_1N_1 \\ {}_2N_1 \end{pmatrix} = \begin{pmatrix} N_{1a} + N_{1b} \\ {}_1N_{1a} + {}_1N_{1b} \\ {}_2N_{1a} + {}_2N_{1b} \end{pmatrix}.$$

The double coset representative matrix element is determined by carrying out the indicated matrix product

$$\begin{bmatrix} \lambda & \begin{pmatrix} \lambda_1 \\ {}_1\lambda_1 \\ {}_2\lambda_1 \end{pmatrix} & \lambda_{1a} & \lambda_{1b} & \lambda_2 \\ {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_{1a} & {}_1\lambda_{1b} & {}_1\lambda_2 \\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_{1a} & {}_2\lambda_{1b} & {}_2\lambda_2 \end{bmatrix} = \begin{bmatrix} \lambda & \lambda_1 & \lambda_2 \\ {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_2 \\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_2 \end{bmatrix}_q \begin{bmatrix} \lambda_1 & \lambda_{1b} & \lambda_2 \\ {}_1\lambda_1 & {}_1\lambda_{1a} & {}_1\lambda_{1b} \\ {}_2\lambda_1 & {}_2\lambda_{1a} & {}_2\lambda_{1b} \end{bmatrix}_p \begin{bmatrix} \lambda_2 & \lambda_2 & 0 \\ {}_1\lambda_2 & {}_1\lambda_2 & 0 \\ {}_2\lambda_2 & {}_2\lambda_2 & 0 \end{bmatrix}_p, \tag{A1}$$

where the labels in curved brackets are the intermediate coupling labels. The delta factors remain as usual and are not indicated here. The last factor on the right which has unit value has been included only to emphasize that the frequency is

$$d_{qp} = d_p = {}_1N_{1a}!\,{}_1N_{1b}!\,{}_1N_2!\,{}_2N_{1a}!\,{}_2N_{1b}!\,{}_2N_2!,$$

as it should be. It is interesting to note that the contraction step can be analyzed using the diagramatic techniques[16] customarily applied to recoupling transformations of $SU(2)$ and for Eq. (A1) gives the ten vertex diagram which results in the product of the two corresponding $(9-j)$ symbols.

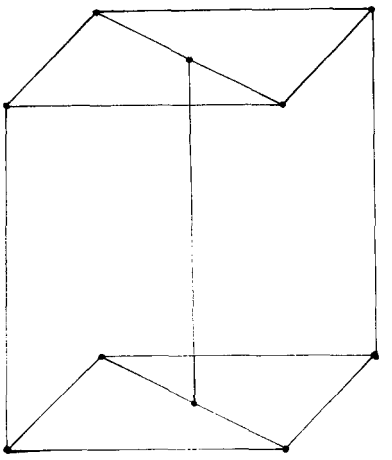

FIG. 1.

Any $m \times m'$ double coset symbol may thus be contracted in successive steps so as to be expressed in the fundamental 2×2 double coset symbols ($9f$). For example, the 3×3 double coset representative matrix element associated with the decomposition

$$S_N = \bigcup_q S_{{}_{1a}N\otimes{}_{1b}N\otimes{}_2N}\, q\, S_{N_{1a}\otimes N_{1b}\otimes N_2}$$

is a sum of the products of four 2×2 double coset representative matrix elements

$$\begin{bmatrix} \lambda & \lambda_1 & \lambda_{1a} & \lambda_{1b} & \lambda_2 \\ {}_1\lambda & & {}_1\lambda_{1a} & {}_1\lambda_{1b} & {}_1\lambda_2 \\ {}_{1a}\lambda & {}_{1a}\lambda_1 & {}_{1a}\lambda_{1a} & {}_{1a}\lambda_{1b} & {}_{1a}\lambda_2 \\ {}_{1b}\lambda & {}_{1b}\lambda_1 & {}_{1b}\lambda_{1a} & {}_{1b}\lambda_{1b} & {}_{1b}\lambda_2 \\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_{1a} & {}_2\lambda_{1b} & {}_2\lambda_2 \end{bmatrix} = \sum_{{}_1\lambda_1} \begin{bmatrix} {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_2 \\ {}_{1a}\lambda & {}_{1a}\lambda_1 & {}_{1a}\lambda_2 \\ {}_{1b}\lambda & {}_{1b}\lambda_1 & {}_{1b}\lambda_2 \end{bmatrix} \begin{bmatrix} {}_1\lambda_1 & {}_1\lambda_{1a} & {}_1\lambda_{1b} \\ {}_{1a}\lambda_1 & {}_{1a}\lambda_{1a} & {}_{1a}\lambda_{1b} \\ {}_{1b}\lambda_1 & {}_{1b}\lambda_{1a} & {}_{1b}\lambda_{1b} \end{bmatrix} \times \begin{bmatrix} \lambda & \lambda_1 & \lambda_2 \\ {}_1\lambda & {}_1\lambda_1 & {}_1\lambda_2 \\ {}_2\lambda & {}_2\lambda_1 & {}_2\lambda_2 \end{bmatrix} \begin{bmatrix} \lambda_1 & \lambda_{1a} & \lambda_{1b} \\ {}_1\lambda_1 & {}_1\lambda_{1a} & {}_1\lambda_{1b} \\ {}_2\lambda_1 & {}_2\lambda_{1a} & {}_2\lambda_{1b} \end{bmatrix} \tag{A2}$$

with frequency

$$d_q = {}_{1a}N_{1a}!\,{}_{1a}N_{1b}!\,{}_{1a}N_2!\,{}_{1b}N_{1a}!\,{}_{1b}N_{1b}!\,{}_{1b}N_2!\,{}_2N_{1a}!\,{}_2N_{1b}!\,{}_2N_2!$$

and corresponds to a sixteen vertex diagram.

A special case[2] of partitions into two or more parts occurs when the subgroup sequence includes several equal parts say $S_{nM} \supset \otimes (S_M)^n$. Instead of proceeding by binary contractions one may introduce as an intermediate subgroup the normalizer $S_{nM} \supset S_n \circledS (S_M)^n$, where the symbol $\circledS$ indicates a semidirect product, and use its irreducible representations to label the states. The theory of little groups may be employed. For an irreducible representation $\{\lambda_j\} j = 1, \cdots, n$ of $(S_M)^n$ the normalizer has a little group $S_{n'} \circledS (S_M)^n$, where $S_n \supset S_{n'}$, such that under conjugation by an element of the little group the irreducible representation is invariant. That is $S_{n'}$ is the subgroup of S_n that permutes equivalent irreducible representations occurring in the set $\{\lambda_j\}$, while the star

or orbit includes all sets $\{\lambda_j\}$ related by the permutations of S_n. The irreducible representation labels of the little groups are sufficient to characterize the irreducible representations of the normalizer subgroup $S_n \circledS (S_M)^n$. Generating the irreducible representation labels of the little groups from the sets $\{\lambda_j\}$ corresponds to applying the operation of plethysm[17] to those representations that are equivalent. The additional label afforded by the plethysm operation may simply be addended to the row or column label involved. That such classification is helpful in resolving some multiplicities is clear from the example

$$\begin{bmatrix} {}_{(1^2)}(3,2,1)_{(2)} & (2,1) & (2,1) \\ (2,1) & {}_1\lambda_1 & {}_1\lambda_2 \\ (2,1) & {}_2\lambda_1 & {}_2\lambda_2 \end{bmatrix}$$

which has a unique meaning for any set ${}_i\lambda_j$. In the unitary group the operation of plethysm corresponds to taking symmetrized inner products and addending this label to those of the Clebsch–Gordan coefficients. Besides the formal resolution of some multiplicities, this manner of proceeding is important for cluster models involving equivalent but distinct groupings in nuclei, atoms, and molecules.

The fundamental multiplicity problem occurs when the outer product of two irreducible representations contains an irreducible representation two or more times and this is not resolvable by a plethysm [e.g., $(3,1).(2,1^2) \supset 2(4,2,1^2)$]. An additional index must be used to distinguish distinct but equivalent irreducible representations. One may give some structural significance to this added index by requiring the basis set being considered to have some fixed relation (i.e., a fixed recoupling transformation) to an equivalent unique basis set. Such sets of unique labels are always possible by sequential reductions by two or one elements[18] (nodes). Some consistent indexing of the multiplicities is assumed in all the relations given here.

APPENDIX B: CYCLE STRUCTURE OF THE DOUBLE COSET REPRESENTATIVE AND ITS PARITY[2]

A double coset has neither unique parity nor cycle structure. However, one may select the double coset representative to correspond to a unique cycle structure. For particular sets ${}_iN$ and N_j let ${}_iN_j^0 \equiv {}_iN \cap N_j$. The identity permutation as a double coset representative can be associated with the double coset symbol $\begin{bmatrix} N & N_j \\ {}_iN & {}_iN_j & 0 \end{bmatrix}$. The transposition of α elements between the subsets ${}_iN_j^0$ and ${}_kN_l^0$ $(i \neq k, j \neq l)$ can be associated with a double coset symbol with indices modified in the $\begin{pmatrix} ij & il \\ kj & kl \end{pmatrix}$ positions by

$$\begin{pmatrix} {}_iN_j & {}_iN_l \\ {}_kN_j & {}_kN_l \end{pmatrix} \equiv \begin{pmatrix} {}_iN_j^0 & {}_iN_l^0 \\ {}_kN_j^0 & {}_kN_l^0 \end{pmatrix} - \alpha \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Similarly, a cyclic permutation of β elements between the subsets ${}_iN_j^0 \to {}_kN_l^0 \to {}_mN_n^0 \to {}_iN_j^0$ can be associated with a double coset symbol with indices in the $(i,k,m)\begin{pmatrix} j \\ l \\ n \end{pmatrix}$ positions modified by $-\beta \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$.

For a given double coset symbol one may proceed as follows: Start with a position with minimum value $|{}_iN_j - {}_iN_j^0|$ and the next smallest such number in the same row or column but with the difference ${}_iN_j - {}_iN_j^0$ opposite in sign to that of the original position. These positions are reduced by the array $|{}_iN_j - {}_iN_j^0|_{\min}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$ and a 2-cycle ${}_2|{}_iN_j - {}_iN_j^0|$ is associated with the double coset representative. By proceeding by iteration, any double coset symbol may be systematically reduced with the introduction of at most $(m-1)(m'-1)$ parameters and the double coset representative is expressed in canonical (disjoint cycles) form, e.g.,

$$\begin{bmatrix} N & N_1 & N_2 \\ {}_1N & {}_1N_1^0 - j & {}_1N_2^0 + j \\ {}_2N & {}_2N_1^0 + j & {}_2N_2^0 - j \end{bmatrix} \text{ has parity } j, \qquad \begin{bmatrix} N & N_1 & N_2 & N_3 \\ {}_1N & {}_1N_1^0 - j - k & {}_1N_2^0 + j & {}_1N_3^0 + k \\ {}_2N & {}_2N_1^0 + j + k & {}_2N_2^0 - j & {}_2N_3^0 - k \end{bmatrix} \text{ has parity } j + k, \text{ and}$$

$$\begin{bmatrix} N & N_1 & N_2 & N_3 \\ {}_1N & {}_1N_1^0 - j - k - m & {}_1N_2^0 + j + m & {}_1N_3^0 + k \\ {}_2N & {}_2N_1^0 + j & {}_2N_2^0 - j - l - m & {}_2N_3^0 + l + m \\ {}_3N & {}_3N_1^0 + k + m & {}_3N_2^0 + l & {}_3N_3^0 - k - l - m \end{bmatrix} \text{ has parity } j + k + l.$$

APPENDIX C: PHASES

We have not examined the question of phase in detail, but the convention advanced by Baird and Biedenharn[19] which can be put in the form

$$\lambda \equiv ({}^1\lambda, {}^2\lambda, \cdots, {}^n\lambda), \qquad P_n(\lambda) \equiv \frac{1}{2} \sum_{i<j}^{n} ({}^i\lambda - {}^j\lambda) \tag{C1}$$

seems appropriate for three reasons.

1. It reduces to the standard convention used for $n = 2$.

2. The phase associated with the Clebsch–Gordan coefficient coupling ${}_1\lambda$ and ${}_2\lambda$ to give $\lambda, P_n({}_1\lambda) - P_n({}_2\lambda)$ is independent of the dimension n[7] and therefore appropriate for couplings in the symmetric group.

3. The resultant phase associated with a transposition of two rows or columns of the double coset representative matrix element is the product of all the phases involved as is the case for $SU(2)$. This is consistent with the association of representations with respect to the alternating group by $\tilde{\lambda} = (1^N) \boxtimes \lambda$. The double coset representative matrix elements for the totally symmetric and the antisymmetric irreducible representations both have even parity under transpositions of rows or

columns. The phases for the two representations are

$$\begin{bmatrix} N & N_j \\ {}_iN & {}_iN_j \end{bmatrix} : (-1)^{\sum_{i,j} {}_iN_j/2} = (-1)^{2N} = 1$$

and

$$\begin{bmatrix} 1^N & 1^{N_j} \\ 1^{{}_iN} & 1^{{}_iN_j} \end{bmatrix} : (-1)^{[\sum_{i,j} {}_iN_j(n-{}_iN_j)]/2} = \{(-1)^{\sum_{i,j} {}_iN_j{}^2}\}^{1/2} = (-1)^{\sum_{i,j} {}_iN_j/2} = 1, \quad \text{(C2)}$$

where n is a dimension so that $n - {}_iN_j \geq 0$ and the sums are over all N.

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Differential equations for one-loop generalized Feynman integrals

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(Receive 21 July 1972)

A system of $(2^N - 1)$ first-order linear homogeneous differential equations in each variable is derived for the generalized (with Speer λ parameters) Feynman integrals corresponding to the one-loop graph with N external lines. This system of differential equations is shown to belong to the class studied by Lappo-Danilevsky. A connection with the matrix representation of the monodromy group in all variables is pointed out.

1. INTRODUCTION

During the last years the analytic properties of Feynman relativistic amplitudes (FRA) have been the object of wide investigation. One may broadly classify these efforts according to the technical devices which have been used for the purpose: (a) homological methods,[1-4] (b) differential equations,[5-8] (c) monodromy groups.[9-13]

The ground for these systematic analyses was prepared by a host of exploratory investigations[14,15] which sprang from the pioneering work of Landau.[16] They were mostly devoted to study the geometrical features of the singular varieties L of increasingly complex classes of graphs and the attached singularities.

The methods of algebraic topology[1,2] pointed out in a rigorous fashion that FRA can be analytically continued in all variables along any path which does not cross L; moreover, FRA were shown to be suitable generalizations of hypergeometric functions (see Sec. 2). As such, two procedures were devised[6] to characterize exhaustively the analyticity of FRA: either by studying their differential properties or by constructing directly the corresponding fundamental group of Poincaré and its matrix representations. The two approaches are in principle equivalent, although the second one has led so far to the most comprehensive results, as it appears from the quoted literature.

The present paper is an attempt to provide a bridge between the two procedures for the particular class of generalized one-loop FRA with N external lines. In fact it will become apparent that the differential equations satisfied by these FRA provide a straightforward procedure to characterize analyticity. Then the direct construction of the Poincaré fundamental group will be avoided and its matrix representation supplied by the structure of the differential system itself.

In Sec. 2 we give the basic notations and recall the main properties of the class of FRA we are considering. In Sec. 3, by choosing suitable values of Speer λ parameters, we define a set of $(2^N - 1)$ one-loop FRA and show they satisfy a system of linear homogeneous differential equations in each variable $s_{i,j}$, with rational coefficients. In Sec. 4 we analyze in detail the singularity structure of this system.

In Sec. 5 we sketch how the explicit solution of the Poincaré problem given by Lappo-Danilevsky[17] applies to our differential system to yield in principle the monodromy group of FRA in each single variable $s_{i,j}$, in addition to a convergent series expansion for the solutions of the differential system. We also point out a factorization property of the coefficients of the differential system which leads to remarkable reductions in said series expansions. Finally, we find the relation between the basic parameters of the representation theory of Ref. 11′ and the present approach.

2. DEFINITIONS AND BASIC PROPERTIES

For convenience we define

$$\mathcal{P} = \{1, 2, \ldots, N\}, \quad \mathcal{R} = \{N+1\} \cup \mathcal{P}, \quad \mathcal{R}_0 = \mathcal{R} \cup \{0\}, \quad N \geq 2 \text{ integer.} \tag{2.1}$$

According to Ref. 11′, we consider the integral

$$F(\mathbf{s}, \boldsymbol{\lambda}) = \int_{\gamma_0} {}^{N-1}\eta \left(\prod_{i \in \mathcal{R}} \alpha_i^{\lambda_i} \right) [D(\alpha, \mathbf{s})]^{-\mu} \tag{2.2a}$$

where

$${}^{N-1}\eta = \sum_{i \in \mathcal{P}} (-1)^i \alpha_i d\alpha_1 d\alpha_2 \cdots d\alpha_{i-1} d\alpha_{i+1} \cdots d\alpha_N \tag{2.2b}$$

and

$$\alpha_{N+1} = -\sum_{i \in \mathcal{P}} \alpha_i, \tag{2.2c}$$

$$D(\alpha, \mathbf{s}) = -\sum_{j>i=1}^{N+1} \alpha_i \alpha_j s_{i,j}, \tag{2.2d}$$

$$2\mu = N + \sum_{i \in \mathcal{R}} \lambda_i. \tag{2.2e}$$

The Speer λ parameters and the $N(N+1)/2$ variables $s_{i,j}$ are supposed complex and independent. It is convenient to define also

$$\begin{cases} s_{i,j} = s_{j,i}, & i > j, \quad \{i,j\} \subset \mathcal{R}, \\ s_{i,i} = 0, & i \in \mathcal{R}_0, \\ s_{0,i} = s_{i,0} = 1, & i \in \mathcal{R}, \end{cases} \tag{2.3}$$

so that a complete $(N+2)\times(N+2)$ Cayley matrix $\|s_{i,j}\|$, $(i,j\in\mathcal{R}_0)$, is formed. The integration in Eq. (2.2a) is performed over a cycle γ_0 in the complex space of the α's, such that the integrand is regular on γ_0.

The variables $s_{i,j}$ are related to $A_{i,j}$ of Ref. 11′ as follows:

$$s_{i,N+1}=A_{i,i},\quad i\in\mathcal{P},$$
$$s_{i,j}=A_{i,i}+A_{j,j}-2A_{i,j},\ \{i,j\}\subset\mathcal{P}, \tag{2.4}$$

so that

$$D(\alpha,\mathbf{s})=\sum_{i,j=1}^{N}\alpha_i\alpha_j A_{i,j}. \tag{2.5}$$

$F(\mathbf{s},\boldsymbol{\lambda})$ is known to be singular on a reducible algebraic variety $L=\cup_{\mathcal{Q}}L_{\mathcal{Q}}$ where the irreducible components are:

$$L_{\mathcal{Q}}=\left\{\mathbf{s}:\binom{\mathcal{Q}}{\mathcal{Q}}=0,\ \mathcal{Q}\subset\mathcal{R},\ 0\leqslant|\mathcal{Q}|\leqslant N-1\right\}; \tag{2.6}$$

$|\mathcal{Q}|$ denotes the number of elements in $\mathcal{Q}$ and $\binom{\mathcal{Q}}{\mathcal{Q}}$ is the determinant of the matrix obtained from $\|s_{i,j}\|$, $(i,j\in\mathcal{R}_0)$, by deleting rows and columns whose indices belong to $\mathcal{Q}$.

Notice that, $\forall\{i,j\}\subset\mathcal{R}$, $L_{\mathcal{Q}}$ is of degree 2 in $s_{i,j}$ if $|\mathcal{Q}|<N-1$ and of degree 1 if $|\mathcal{Q}|=N-1$, provided $\mathcal{Q}\subseteq\mathcal{R}-\{i,j\}$; if $\mathcal{Q}\cap\{i,j\}\neq\phi$, then $\binom{\mathcal{Q}}{\mathcal{Q}}$ does not depend on $s_{i,j}$. Therefore, the number of intersections with L of the line $l_{i,j}=\{s_{i,j}\in\mathbf{C}, s_{h,k}=\text{const}, \forall\{h,k\}\neq\{i,j\}\}$ is

$$K=2\sum_{i=0}^{N-2}\binom{N-1}{i}+1=2^N-1. \tag{2.7}$$

We shall denote with $s^{\pm}_{i,j}(\mathcal{Q})$ the values of $s_{i,j}$ on $L_{\mathcal{Q}}\cap l_{i,j}$, setting of course $s^{+}_{i,j}(\mathcal{R}-\{i,j\})\equiv s^{-}_{i,j}(\mathcal{R}-\{i,j\})$.

Owing to the nature of its singularities, $F(\mathbf{s},\boldsymbol{\lambda})$ can be analytically continued in $\mathbf{S}\equiv\mathbf{C}^{N(N+1)/2}-L$, where $\mathbf{C}^{N(N+1)/2}=\{s_{i,j}:s_{i,j}\in\mathbf{C},\{i,j\}\subset\mathcal{R}\}$, and is a generalized hypergeometric function in the following sense: there are M loops $\gamma_i\subset\mathbf{S}$ with base point $\mathbf{s}^{(0)}$ such that, denoting with F_i the analytic continuation of F from $\mathbf{s}^{(0)}$ to $\mathbf{s}^{(0)}$ along γ_i and with $F_{i,\gamma}$ the analytic continuation of F_i from $\mathbf{s}^{(0)}$ to $\mathbf{s}^{(0)}$ along any other loop $\gamma\subset\mathbf{S}$, we have in a neighborhood of $\mathbf{s}^{(0)}$ not intersecting L

$$F_{i,\gamma}=\sum_{j=1}^{M}\mathcal{L}'_{ji}(\gamma)F_j,\quad i=1,2,\ldots,M, \tag{2.8}$$

where $\mathcal{L}'_{ji}(\gamma)$ are constant with respect to $\mathbf{s}^{(0)}$. As is well known,[6] these properties imply that $F(\mathbf{s},\boldsymbol{\lambda})$ satisfies to a Mth-order linear homogeneous differential equation in any $s_{i,j}$.

In Ref. 11′ a presentation of the Poincaré fundamental group $\pi_1(\mathbf{S},\mathbf{s}^{(0)})$ is explicitly given and its $M\times M$ matrix representation $\mathcal{L}'$ constructed. It turns out that $M=2^N-1$ and that for all generators γ_i of π_1

$$\mathcal{L}'(\gamma_i)-\mathbf{I}=\mathbf{u}(i)\otimes\mathbf{v}(i), \tag{2.9}$$

where $\mathbf{u}(i),\mathbf{v}(i)$ are M- vectors and $\mathbf{I}$ is the identity matrix.

3. SYSTEM OF DIFFERENTIAL EQUATIONS FOR $F(\mathbf{s},\boldsymbol{\lambda})$

Suitable notation is required to handle differentiation of $F(\mathbf{s},\boldsymbol{\lambda})$ with respect to any $s_{i,j}$. We define

$$F(0,l_1,l_2,\ldots,l_{N+1})=\int_{\gamma_0}\eta^{N-1}\left(\prod_{h\in\mathcal{R}}\alpha_h^{\lambda_h+l_h}\right)[D(\alpha,\mathbf{s})]^{-\mu'}, \tag{3.1}$$

where $\mu'=\mu+\frac{1}{2}\sum_{h\in\mathcal{R}}l_h$, each l_h being a signed integer; clearly $F(0,0,\ldots,0)=F(\mathbf{s},\boldsymbol{\lambda})$.

Then we define the function

$$F(1,l_1,l_2,\ldots,l_{N+1})=-\frac{\lambda_{N+1}+l_{N+1}}{\mu+\frac{1}{2}(\sum_{h\in\mathcal{R}}l_h-1)}\times F(0,l_1,l_2,\ldots,l_N,l_{N+1}-1)$$
$$-\sum_{h\in\mathcal{P}}s_{N+1,h}F(0,l_1,\ldots,l_{h-1},l_h+1,l_{h+1},\ldots,l_{N+1}). \tag{3.2}$$

It is also convenient to use the alternative notation:

$$F[\mathcal{Q}_{k_1},\mathcal{Q}_{k_2},\cdots]=F(l_0,l_1,\ldots,l_{N+1}), \tag{3.3a}$$

where

$$\begin{cases}l_0=0,1,\\ \mathcal{Q}_k=\{h:h\in\mathcal{R}_0,l_h=k\},\\ k_p<k_q\ \text{if}\ p<q.\end{cases} \tag{3.3b}$$

We prove then the basic relations:

$$\sum_{k\in\mathcal{R}}F[\{\mathcal{R}_0-\{k\}\}_0,\{k\}_1]=0, \tag{3.4a}$$

$$\sum_{k\in\mathcal{R}_0}s_{h,k}F[\{\mathcal{R}_0-\{k\}\}_0,\{k\}_1]=-\frac{2\lambda_h}{2\mu-1}F[\{h\}_{-1},\{\mathcal{R}_0-\{h\}\}_0],\ h\in\mathcal{R}. \tag{3.4b}$$

Proof: Equation (3.4a) follows from Eq. (2.2c). If $h=N+1$, Eq. (3.4b) coincides with definition (3.2) in the particular case: $l_h=0,\forall h\in\mathcal{R}$. If $h\in\mathcal{P}$, we use the following identity [Eq. (9) of Ref. 6]:

$$\eta^{N-1}\left(\sum_{h\in\mathcal{P}}H_h(\alpha)\frac{\partial D(\alpha,\mathbf{s})}{\partial\alpha_h}\right)[D(\alpha,\mathbf{s})]^{-\nu-1}$$
$$=\nu^{-1}\eta^{N-1}\left(\sum_{h\in\mathcal{P}}\frac{\partial H_h(\alpha)}{\partial\alpha_h}\right)[D(\alpha,\mathbf{s})]^{-\nu}+d\omega, \tag{3.5}$$

where $H_h(\alpha)$, $(h\in\mathcal{P})$, are homogeneous in α's of degree $2\nu-N+1$, d denotes exterior differentiation and ω is a differential $(N-2)$-form. Set $\nu=\mu-\frac{1}{2}$; choose, for any $h\in\mathcal{P}$,

$$H_h(\alpha)=\prod_{p\in\mathcal{R}}(\alpha_p)^{\lambda_p},$$
$$H_k(\alpha)=0,\quad\forall k\in\mathcal{P}-\{h\},$$

and integrate both sides of Eq. (3.5) over the cycle γ_0. As the boundary $\partial\gamma_0$ is empty, Stokes' theorem implies

$$\int_{\gamma_0}d\omega=\int_{\partial\gamma_0}\omega=0.$$

We deduce then that

$$\sum_{k\in\mathcal{R}}(s_{h,k}-s_{N+1,k})F[\{\mathcal{R}_0-\{k\}\}_0,\{k\}_1]$$

$$= -\frac{2\lambda_h}{2\mu-1} F[\{h\}_{-1},\{\mathcal{R}_0 - \{h\}\}_0] + \frac{2\lambda_{N+1}}{2\mu-1} F[\{N+1\}_{-1},\{\mathcal{R}_0 - \{N+1\}\}_0], \forall h \in \mathcal{P}.$$

By adding this equation to Eq. (3.4b) in the case $h = N + 1$, we obtain Eq. (3.4b) for the case $h \in \mathcal{P}$.

We remark that the matrix of coefficients in the lhs of Eqs. (3.4a) and (3.4b) coincides with the Cayley matrix $\| s_{i,j} \|$, $(i, j \in \mathcal{R}_0)$. It is worth exemplifying this linear system in the case $N = 2$; it reads, using the notation (3.1),

$$F(0,1,0,0) + F(0,0,1,0) + F(0,0,0,1) = 0,$$

$$F(1,0,0,0) + s_{1,2}F(0,0,1,0) + s_{1,3}F(0,0,0,1) = -\frac{2\lambda_1}{2\mu-1} F(0,-1,0,0),$$

$$F(1,0,0,0) + s_{2,1}F(0,1,0,0) + s_{2,3}F(0,0,0,1) = -\frac{2\lambda_2}{2\mu-1} F(0,0,-1,0), \quad (3.6)$$

$$F(1,0,0,0) + s_{3,1}F(0,1,0,0) + s_{3,2}F(0,0,1,0) = -\frac{2\lambda_3}{2\mu-1} F(0,0,0,-1).$$

As we shall soon have to consider the determinants of submatrices of $\| s_{h,k} \|$, $(h, k \in \mathcal{R}_0)$, we introduce the notation

$$\begin{pmatrix} \mathcal{A}, p_1, p_2, \ldots, p_r \\ \mathcal{A}, q_1, q_2, \ldots, q_r \end{pmatrix}, \quad (3.7)$$

where

$$\mathcal{A} \equiv \{a_1, a_2, \ldots, a_{|\mathcal{A}|}\} \subset \mathcal{R},$$
$$p_i, q_i \in \mathcal{R} - \mathcal{A}, \quad (i = 1, 2, \ldots, r), \quad (3.8)$$
$$p_h \neq p_k, \quad q_h \neq q_k \quad \text{if } h \neq k.$$

In (3.7), $\binom{\mathcal{A}, p_1, p_2, \ldots, p_r}{\mathcal{A}, q_1, q_2, \ldots, q_r}$ is the determinant of the matrix obtained from $\| s_{h,k} \|$, $(h, k \in \mathcal{R}_0)$, by deleting rows and columns whose indices belong to $\mathcal{A} \cup \{p_1, p_2, \ldots, p_r\}$ and to $\mathcal{A} \cup \{q_1, q_2, \ldots, q_r\}$ respectively, multiplied by the sign $(-1)^\sigma$, where

$$\sigma = \sum_{l=1}^{r} (p_l + q_l) + \sigma_p + \sigma_q,$$

σ_p being 0 and 1 according to whether $(a_1, a_2, \ldots, a_{|\mathcal{A}|}, p_1, p_2, \ldots, p_r)$ is an even or odd permutation of $\mathcal{A} \cup \{p_1, p_2, \ldots, p_r\}$ with respect to the one where the elements are arranged in increasing order; similarly for σ_q.

We may now state:

Theorem 3.9: The set of $(2^N - 1)$ **FRA**

$$F_{\mathcal{A}} = F[\{\mathcal{R}_0 - \mathcal{A}\}_0, \mathcal{A}_1], \quad \mathcal{A} \in \Omega \equiv \{\mathcal{B} : \mathcal{B} \subseteq \mathcal{R}, |\mathcal{B}| > 0, |\mathcal{B}| = 0 \bmod 2\} \quad (3.9)$$

satisfy, for every $\{i, j\} \subset \mathcal{R}$, a system of $(2^N - 1)$ differential equations of the type:

$$\frac{\partial F_{\mathcal{A}}}{\partial s_{i,j}} = \sum_{\mathcal{B} \in \Omega} R^{(i,j)}_{\mathcal{B},\mathcal{A}} F_{\mathcal{B}}, \quad (3.10)$$

where $R^{(i,j)}_{\mathcal{B},\mathcal{A}}$ are rational functions of $s_{i,j}$ with poles at $s^{\pm}_{i,j}(\mathcal{C})$ for suitable $\mathcal{C} \subseteq \mathcal{R} - \{i, j\}$.

Proof: From Eqs. (3.1) and (3.3) we derive

$$\frac{\partial F_{\mathcal{A}}}{\partial s_{i,j}} = \left(\mu + \frac{|\mathcal{A}|}{2}\right) F_{\mathcal{A} \cup \{i,j\}}, \quad \text{if} \quad \{i, j\} \subset \mathcal{R} - \mathcal{A}, \quad (3.11a)$$

$$= \left(\mu + \frac{|\mathcal{A}|}{2}\right) F[\{\mathcal{R}_0 - \mathcal{A} - \{i\}\}_0, \{(\mathcal{A} \cup \{i\}) - \{j\}\}_1, \{j\}_2], \quad \text{if} \quad i \in \mathcal{R} - \mathcal{A}, j \in \mathcal{A}, \quad (3.11b)$$

$$= \left(\mu + \frac{|\mathcal{A}|}{2}\right) F[\{\mathcal{R}_0 - \mathcal{A}\}_0, \{\mathcal{A} - \{i, j\}\}_1, \{i, j\}_2], \quad \text{if} \quad \{i, j\} \subset \mathcal{A}. \quad (3.11c)$$

As $\mathcal{A} \cup \{i, j\} \in \Omega$, Eq. (3.11a) already has the form (3.10).

To deal with (3.11b), we choose any $\mathcal{B} \subseteq \mathcal{R}$, $|\mathcal{B}| = 1 \bmod 2$, and select, from the system (3.4), Eq. (3.4a) and Eqs. (3.4b) with $h \in \mathcal{B}$; from these equations, increasing every l_k, $k \in \mathcal{B}$, by one unit, we get

$$\sum_{k \in \mathcal{B}} s_{0,k} F[\{\mathcal{R}_0 - \mathcal{B}\}_0, \{\mathcal{B} - \{k\}\}_1, \{k\}_2] = -\sum_{k \in \mathcal{R} - \mathcal{B}} s_{0,k} F_{\mathcal{B} \cup \{k\}}, \quad (3.12a)$$

$$s_{h,0} F[\{\mathcal{R} - \mathcal{B}\}_0, \{\mathcal{B} \cup \{0\}\}_1] + \sum_{k \in \mathcal{B}} s_{h,k} F[\{\mathcal{R}_0 - \mathcal{B}\}_0, \{\mathcal{B} - \{k\}\}_1, \{k\}_2] = -\sum_{k \in \mathcal{R} - \mathcal{B}} s_{h,k} F_{\mathcal{B} \cup \{k\}} - \frac{2\lambda_h + 2}{2\mu + |\mathcal{B}| - 1} F_{\mathcal{B} - \{h\}}, \quad \forall h \in \mathcal{B}. \quad (3.12b)$$

This system can be solved to yield

$$\binom{\mathcal{R} - \mathcal{B}}{\mathcal{R} - \mathcal{B}} F[\{\mathcal{R}_0 - \mathcal{B}\}_0, \{\mathcal{B} - \{k\}\}_1, \{k\}_2] = \sum_{h \in \mathcal{R} - \mathcal{B}} \binom{\mathcal{R} - \mathcal{B} - \{h\}, h}{\mathcal{R} - \mathcal{B} - \{h\}, k} F_{\mathcal{B} \cup \{h\}} - \sum_{h \in \mathcal{B}} \frac{2\lambda_h + 2}{2\mu + |\mathcal{B}| - 1} \binom{\mathcal{R} - \mathcal{B}, h}{\mathcal{R} - \mathcal{B}, k} F_{\mathcal{B} - \{h\}}, \quad \forall k \in \mathcal{B}, \quad (3.13)$$

with the convention that, if $|\mathcal{B}| = 1$, the second term in the rhs has to be neglected as $\binom{\mathcal{R}}{\mathcal{R}} = 0$. Choosing $\mathcal{B} = \mathcal{A} \cup \{i\}$, $k = j \in \mathcal{A}$, we are through with case (3.11b).

To deal with the case (3.11c), we select, from the system (3.4), Eq. (3.4a) and Eqs. (3.4b) labelled by $h \in \mathcal{A}$; after having increased by one unit each l_k, $k \in \mathcal{A} - \{i\}$, and by two units l_i, they read

$$s_{h,0} F[\{\mathcal{R} - \mathcal{A}\}_0, \{(\mathcal{A} - \{i\}) \cup \{0\}\}_1, \{i\}_2] + s_{h,i} F[\{\mathcal{R}_0 - \mathcal{A}\}_0, \{\mathcal{A} - \{i\}\}_1, \{i\}_3] + \sum_{k \in \mathcal{A} - \{i\}} s_{h,k} F[\{\mathcal{R}_0 - \mathcal{A}\}_0, \{\mathcal{A} - \{i, k\}\}_1, \{i, k\}_2] = -\sum_{k \in \mathcal{R} - \mathcal{A}} s_{h,k} F[\{\mathcal{R}_0 - \mathcal{A} - \{k\}\}_0, \{(\mathcal{A} - \{i\}) \cup \{k\}\}_1, \{i\}_2] - \Phi_h, \quad (3.14a)$$

where $h \in \mathfrak{A} \cup \{0\}$ and:

$$\Phi_h = 0 \quad \text{if} \quad h = 0, \tag{3.14b}$$

$$\Phi_h = \frac{2\lambda_i + 4}{2\mu + |\mathfrak{A}|} F_{\mathfrak{A}}, \quad \text{if} \quad h = i, \tag{3.14c}$$

$$\Phi_h = \frac{2\lambda_h + 2}{2\mu + |\mathfrak{A}|} F[\{(\mathfrak{R}_0 - \mathfrak{A}) \cup \{h\}\}_0, \{\mathfrak{A} - \{i,h\}\}_1, \{i\}_2], \quad \text{if} \quad h \in \mathfrak{A} - \{i\}. \tag{3.14d}$$

Notice that the determinant of this linear system is $\binom{\mathfrak{R}-\mathfrak{A}}{\mathfrak{R}-\mathfrak{B}}$. Equations (3.14) can be solved to yield $F[\{\mathfrak{R}_0 - \mathfrak{A}\}_0, \{\mathfrak{A} - \{i,j\}\}_1, \{i,j\}_2]$ in terms of the functions which appear in the rhs. As these functions can be linearly expressed, by means of Eq. (3.13), in terms of $F_{\mathfrak{C}}$, with suitable $\mathfrak{C} \in \Omega$, the proof is completed.

The matrix elements $R^{(i,j)}_{\mathfrak{B},\mathfrak{A}}$, $\{i,j\} \subset \mathfrak{A}$, which can be explicitly computed by solving Eqs. (3.14), are very complicated expressions which we shall quote in suitable form in the following section.

The dimension $(2^N - 1)$ of the vector space spanned by the FRA which appear in Theorem 3.9 agrees with the result of the general theory developed in Ref. 6 when applied to our class of integrals.

4. THE SINGULARITIES OF THE DIFFERENTIAL SYSTEM

The statement of the theorem of the previous section does not specify explicitly which singularities affect a given equation of the system (3.10). To extract from Eqs. (3.13) and (3.14) a complete characterization of such singularities, let us define, for every $\mathfrak{A}$ such that $\mathfrak{A} \cap \{i,j\} \neq \phi$:

$$\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})) = \lim_{s_{i,j} \to s^{\pm}_{i,j}(\mathfrak{C})} \{[s_{i,j} - s^{\pm}_{i,j}(\mathfrak{C})] R^{(i,j)}_{\mathfrak{B},\mathfrak{A}}\} \tag{4.1}$$

$$\mathfrak{C} \subseteq \mathfrak{R} - \{i,j\}, \quad \mathfrak{B} \in \Omega, \mathfrak{A} \in \Omega.$$

By means of the relations

$$s^{\pm}_{i,j}(\mathfrak{C}) = \left\{ \binom{\mathfrak{C}, i}{\mathfrak{C}, j}_{s_{i,j}=0} \pm \left[\binom{\mathfrak{C} \cup \{i\}}{\mathfrak{C} \cup \{i\}} \binom{\mathfrak{C} \cup \{j\}}{\mathfrak{C} \cup \{j\}} \right]^{1/2} \right\} \Big/ \binom{\mathfrak{C} \cup \{i,j\}}{\mathfrak{C} \cup \{i,j\}}, \tag{4.2a}$$

$$\mathfrak{C} \subset \mathfrak{R} - \{i,j\}$$

$$s^{\pm}_{i,j}(\mathfrak{R} - \{i,j\}) = 0, \tag{4.2b}$$

$$\lim_{s_{i,j} \to s^{\pm}_{i,j}(\mathfrak{C})} \left[s_{i,j} - s^{\pm}_{i,j}(\mathfrak{C}) \right] \binom{\mathfrak{C}}{\mathfrak{C}}^{-1} = \frac{1}{2} \left[\binom{\mathfrak{C}, i}{\mathfrak{C}, j}_{s_{i,j} = s^{\pm}_{i,j}(\mathfrak{C})} \right]^{-1}, \tag{4.2c}$$

$$\mathfrak{C} \subseteq \mathfrak{R} - \{i,j\},$$

which can be easily checked using the identities satisfied by Cayley determinants quoted in Refs. 15, a straightforward computation based on Eq. (3.13) and on the explicit solution of the system (3.14), leads to the following results:

$$\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})) = \psi_{\mathfrak{B}}(s^{\pm}_{i,j}(\mathfrak{C})) \cdot \varphi_{\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})), \tag{4.3a}$$

$$\mathfrak{A}, \mathfrak{B} \in \Omega, \ \mathfrak{C} \subseteq \mathfrak{R} - \{i,j\},$$

where the components of ψ, φ are specified by:

(i) $N - |\mathfrak{C}| = 1 \bmod 2$:

$$\psi_{\mathfrak{B}}(s^{\pm}_{i,j}(\mathfrak{C})) = \Bigg\{ \sum_{\{h,k\} \subseteq \mathfrak{B} \cap \mathfrak{C}} \delta_{\mathfrak{C} - \{h,k\} = \mathfrak{R} - \mathfrak{B}} [\mu + \tfrac{1}{2}(N - |\mathfrak{C}| + 1)] \times \binom{\mathfrak{C} - \{h,k\}}{\mathfrak{C} - \{h,k\}} \Big/ \binom{\mathfrak{C} - \{h,k\}, h}{\mathfrak{C} - \{h,k\}, k}$$

$$+ \sum_{\substack{h \in \mathfrak{R} - (\mathfrak{B} \cup \mathfrak{C}) \\ k \in \mathfrak{B} \cap \mathfrak{C}}} \delta_{\mathfrak{C} \cup \{h\} - \{k\} = \mathfrak{R} - \mathfrak{B}} (\lambda_h + 1) \times \binom{\mathfrak{C} \cup \{h\} - \{k\}}{\mathfrak{C} \cup \{h\} - \{k\}} \Big/ \binom{\mathfrak{C} - \{k\}, h}{\mathfrak{C} - \{k\}, k}$$

$$+ \sum_{\{h,k\} \subseteq \mathfrak{R} - (\mathfrak{B} \cup \mathfrak{C})} \delta_{\mathfrak{C} \cup \{h,k\} = \mathfrak{R} - \mathfrak{B}} \frac{(\lambda_h + 1)(\lambda_k + 1)}{\mu + \frac{1}{2}(N - |\mathfrak{C}| - 1)} \times \binom{\mathfrak{C} \cup \{h,k\}}{\mathfrak{C} \cup \{h,k\}} \Big/ \binom{\mathfrak{C}, h}{\mathfrak{C}, k}$$

$$- \delta_{\mathfrak{C} = \mathfrak{R} - \mathfrak{B}} 2 \left(\mu - \sum_{h \in \mathfrak{C}} \lambda_h - |\mathfrak{C}| + 1 \right) \Bigg\}_{s_{i,j} = s^{\pm}_{i,j}(\mathfrak{C})}, \tag{4.3b}$$

$$\varphi_{\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})) = \tfrac{1}{2} \delta_{\mathfrak{C} = \mathfrak{R} - \mathfrak{A}}; \tag{4.3c}$$

(ii) $N - |\mathfrak{C}| = 0 \bmod 2$:

$$\psi_{\mathfrak{B}}(s^{\pm}_{i,j}(\mathfrak{C})) = \Bigg\{ \tfrac{1}{2} \sum_{h \in \mathfrak{B} \cap \mathfrak{C}} \delta_{\mathfrak{C} - \{h\} = \mathfrak{R} - \mathfrak{B}} \binom{\mathfrak{C} - \{h\}, i}{\mathfrak{C} - \{h\}, h} - \sum_{h \in \mathfrak{R} - (\mathfrak{B} \cup \mathfrak{C})} \delta_{\mathfrak{C} \cup \{h\} = \mathfrak{R} - \mathfrak{B}} \frac{\lambda_h + 1}{2\mu + N - |\mathfrak{C}|} \binom{\mathfrak{C}, i}{\mathfrak{C}, h} \Bigg\}_{s_{i,j} = s^{\pm}_{i,j}(\mathfrak{C})}, \tag{4.3d}$$

$$\varphi_{\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})) = \Bigg\{ \sum_{k \in \mathfrak{A} \cap \mathfrak{C}} \delta_{\mathfrak{C} - \{k\} = \mathfrak{R} - \mathfrak{A}} (\lambda_k + 1) \binom{\mathfrak{C} - \{k\}, i}{\mathfrak{C} - \{k\}, k}^{-1} + \tfrac{1}{2} \sum_{k \in \mathfrak{R} - (\mathfrak{A} \cup \mathfrak{C})} \delta_{\mathfrak{C} \cup \{k\} = \mathfrak{R} - \mathfrak{A}} (2\mu + N - |\mathfrak{C}|) \times \binom{\mathfrak{C}, i}{\mathfrak{C}, k}^{-1} \Bigg\}_{s_{i,j} = s^{\pm}_{i,j}(\mathfrak{C})}, \tag{4.3e}$$

where $\delta_{\mathfrak{D}=\mathcal{E}} = 1$ if $\mathfrak{D} = \mathcal{E}$, $\delta_{\mathfrak{D}=\mathcal{E}} = 0$ if $\mathfrak{D} \neq \mathcal{E}$.

It might seem that the index i plays a privileged role in Eqs. (4.3d) and (4.3e), but this is not the case because one can easily verify that the rhs is symmetrical under the exchange $i \leftrightarrow j$.

To make the notations clearer, we like to exemplify the above results in the case $N = 2$ where the $\tilde{\mathbf{U}}$'s are 3×3 matrices; by setting $i = 1, j = 2$, these matrices read

$$\tilde{\mathbf{U}}(s^{\pm}_{1,2}(\phi)) = \begin{array}{c} \\ \{2,3\} \\ \{1,3\} \\ \{1,2\} \end{array} \begin{array}{c} \begin{array}{ccc} \{2,3\} & \{1,3\} & \{1,2\} \end{array} \\ \begin{pmatrix} -\frac{\lambda_1+1}{2} & -\frac{\lambda_1+1}{2}\frac{(\frac{1}{1})}{(\frac{1}{2})} & -\frac{\lambda_1+1}{2}\frac{(\frac{1}{1})}{(\frac{1}{3})} \\ -\frac{\lambda_2+1}{2}\frac{(\frac{1}{2})}{(\frac{1}{1})} & -\frac{\lambda_2+1}{2} & -\frac{\lambda_2+1}{2}\frac{(\frac{1}{2})}{(\frac{1}{3})} \\ -\frac{\lambda_3+1}{2}\frac{(\frac{1}{3})}{(\frac{1}{1})} & -\frac{\lambda_3+1}{2}\frac{(\frac{1}{3})}{(\frac{1}{2})} & -\frac{\lambda_3+1}{2} \end{pmatrix}_{s_{1,2}=s^{\pm}_{1,2}(\phi)} \end{array},$$

$$\tilde{\mathbf{U}}(s^{\pm}_{1,2}(\{3\})) = \begin{array}{c} \\ \{2,3\} \\ \{1,3\} \\ \{1,2\} \end{array} \begin{array}{c} \begin{array}{ccc} \{2,3\} & \{1,3\} & \{1,2\} \end{array} \\ \begin{pmatrix} 0 & 0 & \frac{\lambda_1+1}{2}\frac{(\frac{1}{1})}{(\frac{1}{3})} \\ 0 & 0 & \frac{\lambda_2+1}{2}\frac{(\frac{2}{2})}{(\frac{2}{3})} \\ 0 & 0 & -\mu+\lambda_3 \end{pmatrix}_{s_{1,2}=s^{\pm}_{1,2}(\{3\})} \end{array}$$

We remark that the factorization property (4.3a) strongly reminds us of Eq. (2.9).

5. CONNECTION WITH LAPPO-DANILEVSKY'S THEORY

To show that our differential system belongs to the class considered by Lappo-Danilevsky,[17] we have to cast it into a different form. By means of the definition (4.1), we write Eq. (3.10) as follows:

$$\frac{\partial F_{\mathfrak{A}}}{\partial s_{i,j}} = \left(\mu + \frac{|\mathfrak{A}|}{2}\right) F_{\mathfrak{A}\cup\{i,j\}}, \qquad \forall \mathfrak{A} \in \Omega,\ \mathfrak{A}\cap\{i,j\} = \phi, \tag{5.1a}$$

$$\frac{\partial F_{\mathfrak{A}}}{\partial s_{i,j}} = \sum_{\mathfrak{B}\in\Omega}\left[\frac{\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{R}-\{i,j\}))}{s_{i,j}} + \sum_{\mathfrak{C}\subset\mathfrak{R}-\{i,j\}}\left(\frac{\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{+}_{i,j}(\mathfrak{C}))}{s_{i,j}-s^{+}_{i,j}(\mathfrak{C})} + \frac{\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{-}_{i,j}(\mathfrak{C}))}{s_{i,j}-s^{-}_{i,j}(\mathfrak{C})}\right)\right] F_{\mathfrak{B}},$$

$$\forall \mathfrak{A} \in \Omega, \mathfrak{A}\cap\{i,j\} \neq \phi. \tag{5.1b}$$

Then we make the transformation

$$s_{i,j} = (\alpha x + \beta)/(\gamma x + \delta), \qquad \alpha\delta - \beta\gamma \neq 0, \qquad \alpha,\beta,\gamma \neq 0, \tag{5.2a}$$

so that we may define

$$x_{\infty} = -\delta/\gamma, \tag{5.2b}$$

$$x^{\pm}_{\mathfrak{C}} = -[\delta s^{\pm}_{i,j}(\mathfrak{C}) - \beta]/[\gamma s^{\pm}_{i,j}(\mathfrak{C}) - \alpha], \qquad \mathfrak{C}\subseteq\mathfrak{R}-\{i,j\}. \tag{5.2c}$$

We specify (5.2a) by setting

$$(\alpha\delta - \beta\gamma)/\gamma^2 = 1. \tag{5.2d}$$

From Eqs. (5.1) we obtain, writing $F_{\mathfrak{A}}$, $\mathfrak{A}\in\Omega$, as a one-row matrix $\mathbf{F}$

$$\frac{\partial \mathbf{F}}{\partial x} = \mathbf{F}\left[\frac{\mathbf{U}^{(1)}(\infty)}{x-x_{\infty}} + \frac{\mathbf{U}^{(2)}(\infty)}{(x-x_{\infty})^2} + \frac{\mathbf{U}(0)}{x-x_{\mathfrak{R}-\{i,j\}}} + \sum_{\mathfrak{C}\subset\mathfrak{R}-\{i,j\}}\left(\frac{\mathbf{U}(s^{+}_{i,j}(\mathfrak{C}))}{x-x^{+}_{\mathfrak{C}}} + \frac{\mathbf{U}(s^{-}_{i,j}(\mathfrak{C}))}{x-x^{-}_{\mathfrak{C}}}\right)\right], \tag{5.3}$$

where, $\forall \mathfrak{A},\mathfrak{B}\in\Omega$,

$$(\mathbf{U}(0))_{\mathfrak{B},\mathfrak{A}} = \delta_{\mathfrak{A}\cap\{i,j\}\neq\phi}\,\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{R}-\{i,j\})), \tag{5.4a}$$

$$[\mathbf{U}(s^{\pm}_{i,j}(\mathfrak{C}))]_{\mathfrak{B},\mathfrak{A}} = \delta_{\mathfrak{A}\cap\{i,j\}\neq\phi}\tilde{U}_{\mathfrak{B},\mathfrak{A}}(s^{\pm}_{i,j}(\mathfrak{C})), \mathfrak{C}\subset\mathfrak{R}-\{i,j\}, \tag{5.4b}$$

$$(\mathbf{U}^{(1)}(\infty))_{\mathfrak{B},\mathfrak{A}} = -\Big\{\mathbf{U}(0) + \sum_{\mathfrak{C}\subset\mathfrak{R}-\{i,j\}}[\mathbf{U}(s^{+}_{i,j}(\mathfrak{C})) + \mathbf{U}(s^{-}_{i,j}(\mathfrak{C}))]\Big\}_{\mathfrak{B},\mathfrak{A}}, \tag{5.4c}$$

$$(\mathbf{U}^{(2)}(\infty))_{\mathfrak{B},\mathfrak{A}} = \delta_{\mathfrak{A}\cap\{i,j\}=\phi}\,\delta_{\mathfrak{B}=\mathfrak{A}\cup\{i,j\}}(\mu + |\mathfrak{A}|/2); \tag{5.4d}$$

in Eqs. (5.4a), (5.4b) we used the notation

$$\delta_{\mathfrak{D}\neq\mathcal{E}} = 1 \quad \text{if} \quad \mathfrak{D}\neq\mathcal{E}, \quad \delta_{\mathfrak{D}\neq\mathcal{E}} = 0 \quad \text{if} \quad \mathfrak{D} = \mathcal{E}.$$

First we remark that the differential system (5.3) is regular at $x=\infty$. Secondly, by direct computation from Eqs. (5.4a), (5.4b), and (5.4c) it is possible to verify that $\mathbf{U}^{(1)}(\infty)$ cannot be expressed as $\psi(\infty)\otimes\varphi(\infty)$. This property reflects a corresponding feature of the general results derived in Ref. 11', where the discontinuity operator of the word at infinity does not share the factorization property (2.9) of the generators of the monodromy group.

If we consider the $(2^N-1)\times(2^N-1)$ matrix $\mathbf{Y}(x)$ whose rows correspond to the linearly independent solutions of Eq. (5.3), then said matrix satisfies an equation of the following type:

$$\frac{d\mathbf{Y}(x)}{dx} = \sum_{a=1}^{S}\sum_{b=1}^{M}\frac{\mathbf{Y}(x)\mathbf{U}^{(b)}_{a}}{(x-x_a)^b}, \qquad S, M \geq 1, \tag{5.5}$$

where $\mathbf{U}^{(b)}_{a}$ are constant $(2^N-1)\times(2^N-1)$ matrices.

Some of the Lappo-Danilevsky's results concerning Eq. (5.5) can be summarized (Ref. 17, Mémoire cinquième) as follows: $x_0 \neq x_a$ $(a = 1, 2, \ldots, S)$ having been

chosen, the solution $\mathbf{Y}_{x_0}(x)$ of (5.5), such that $\mathbf{Y}_{x_0}(x_0) = \mathbf{I}$, is

$$\mathbf{Y}_{x_0}(x) = \mathbf{I} + \sum_{n=1}^{\infty} \sum_{a_1,a_2,\ldots,a_n=1}^{S} \sum_{b_1,b_2,\ldots,b_n=1}^{M} \mathbf{U}_{a_1}^{(b_1)} \mathbf{U}_{a_2}^{(b_2)} \cdots \mathbf{U}_{a_n}^{(b_n)} \times L_{x_0}(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_n}^{b_n} | x), \quad (5.6)$$

where

$$L_{x_0}(x_{a_1}^{b_1} | x) = \int_{x_0}^{x} \frac{d\xi}{(\xi - x_{a_1})^{b_1}},$$

$$L_{x_0}(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_n}^{b_n} | x) = \int_{x_0}^{x} \frac{L_{x_0}(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_{n-1}}^{b_{n-1}} | \xi)}{(\xi - x_{a_n})^{b_n}} d\xi, \quad n > 1. \quad (5.7)$$

The expansion (5.6) is uniformly convergent in any finite domain of the complex plane cut from x_a to ∞ ($a = 1, \ldots, S$). As $\mathbf{Y}_{x_0}(x)$ is analytically continued from x_0 to x_0 along a closed path γ_a which encircles anticlockwise only x_a, the final value $\mathbf{V}_a$ of $\mathbf{Y}_{x_0}$ is given by an expansion obtained from (5.6) by replacing $L_{x_0}(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_n}^{b_n} | x)$ with the corresponding analytic continuation:

$$P_a(x_{a_1}^{b_1} | x_0) = \int_{\gamma_a} \frac{d\xi}{(\xi - x_{a_1})^{b_1}},$$

$$P_a(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_n}^{b_n} | x_0) = \int_{\gamma_a} \frac{L_{x_0}(x_{a_1}^{b_1}, x_{a_2}^{b_2}, \ldots, x_{a_{n-1}}^{b_{n-1}} | \xi)}{(\xi - x_{a_n})^{b_n}} d\xi, \quad n > 1. \quad (5.8)$$

The $\mathbf{V}_a$ provide a representation of the monodromy group of the system (5.5) in the variable x and the behavior of $\mathbf{Y}_{x_0}(x)$ in the neighborhood of x_a is given by $\mathbf{Y}_{x_0}(x) = \mathbf{Z}(x)(x - x_a)^{\mathbf{W}_a}$, where $\mathbf{Z}(x)$ is single-valued analytic in said neighborhood and $\mathbf{W}_a$ satisfies

$$\mathbf{W}_a = (1/2\pi i) \log \mathbf{V}_a .$$

We notice that, owing to the factorization property (4.3a), the series expansions for $\mathbf{Y}_{x_0}$ and $\mathbf{V}_a$ simplify remarkably in our particular case. In fact, from (4.3a) it follows that

$$\tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}_1))\tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}_2)) \cdots \tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}_k)) = \text{const}\, \tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}_1))\tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}_k)), \quad (5.9)$$

so that only second order terms in $\tilde{\mathbf{U}}$'s appear in said expansions. It is not difficult to find out the selection rules for the products of type (5.9); however, as the generic expression of the scalar product $\sum_{\mathfrak{a} \in \Omega} \varphi_{\mathfrak{a}}(s_{i,j}^{\pm}(\mathcal{C}_1))\, \psi_{\mathfrak{a}}(s_{i,j}^{\pm}(\mathcal{C}_2))$ is rather complicated by itself, we shall not quote the details.

Finally, we point out the relation between the parameters $X(\chi)$ of Ref. 11′ and the trace of $\tilde{\mathbf{U}}$'s. From Eqs. (4.3) we deduce that

$$\sum_{\mathfrak{a} \in \Omega} [\tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}))]_{\mathfrak{a},\mathfrak{a}} = -\mu + \sum_{h \in \mathcal{C}} \lambda_h + |\mathcal{C}| - \tfrac{1}{2} - \delta,$$

$$\delta = 0 \quad \text{if} \quad N - |\mathcal{C}| = 0 \bmod 2, \qquad \delta = \tfrac{1}{2} \quad \text{if} \quad N - |\mathcal{C}| = 1 \bmod 2. \quad (5.10)$$

Comparing (5.10) with (4.2.0) of Ref. 11′, where we set $\chi = \mathcal{C}$, $s = N - 1$, we find

$$\exp[2\pi i\ \mathrm{Tr}\tilde{\mathbf{U}}(s_{i,j}^{\pm}(\mathcal{C}))] = X(\mathcal{C}). \quad (5.11)$$

This relation provides a link between the representations of the monodromy group in all variables as constructed in Ref. 11′, and those of the monodromy group in each single variable as obtained by means of Lappo-Danilevsky's expansions.

ACKNOWLEDGMENTS

We like to thank Professor T. Regge for his kind interest and for many useful discussions.

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On stochastic scattering

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(Received 7 September 1972)

The Schrödinger equation for two-particle scattering with random potential is considered, including both the cases of a local and a nonlocal potential with convolution kernel. It is shown that the statistical fluctuations of the potential give rise to additional terms which increase the scattering cross section, and an evaluation of the additional terms in the Born approximation is given. A brief discussion about analyticity properties of the scattering amplitude under suitable assumptions is included.

1. INTRODUCTION

We consider the Schrödinger equation for the quantum-mechanical scattering of a nonrelativistic particle of zero spin

$$L_0\psi = U\psi + V\psi \tag{1}$$

where $L_0 = (2m)^{-1}\hbar^2[\nabla^2 + k^2]$, in which ∇^2 is the three-dimensional Laplace operator, $k^2 = 2mE\hbar^{-2}$, E is the (relative) energy, m is the (reduced) mass, and $h = 2\pi\hbar$ is the Planck constant.[1] As usual, U denotes the operator of multiplication by $U(\mathbf{x})$, the deterministic (nonrandom) potential, while the operator V, describing a nonlocal potential, is defined by

$$V\psi = \int_{R^3} W(\mathbf{x}-\mathbf{y})[v(\mathbf{x}) + v^*(\mathbf{y})]\psi(\mathbf{y})d\mathbf{y} \qquad (\mathbf{x},\mathbf{y}\in R^3), \tag{2}$$

where R^3 denotes the familiar Euclidean three-dimensional space, and the asterisk denotes complex conjugation. The Cartesian vector notation will be used, a dot denoting scalar products in R^3.

The following assumptions are made throughout:
(i) The wavefunction ψ is a random function of $\mathbf{x}\in R^3$ with average value $\bar{\psi}(\mathbf{x})$:

$$\psi(\mathbf{x}) = \bar{\psi}(\mathbf{x}) + \varphi(\mathbf{x}), \langle\varphi(\mathbf{x})\rangle = 0, \tag{3}$$

where the bracket denotes statistical averages. Thus, denoting by (Ω, S, P) the underlying probability space of elementary events $\omega\in\Omega$, $\psi(\mathbf{x}) = \psi(\mathbf{x},\omega)$ is a function of $\mathbf{x}$ with values in the Hilbert space $L^2(\Omega)$ of all complex-valued random variables with scalar product defined for any $(\forall)\ \eta_1,\eta_2\in L^2(\Omega)$ by $(\eta_1,\eta_2) = \int_\Omega \eta_1(\omega)\eta_2^*(\omega)dP(\omega)$, and the average is defined by $\langle\psi(\mathbf{x})\rangle = (\psi(\mathbf{x},\omega),1)$. Also $\psi(\mathbf{x},\omega)$ is a bounded function of $\mathbf{x}$ of class $C^2(R^3)$ for P-a.e. $\omega\in\Omega$.[2]

(ii) $W(\mathbf{x})$ is a given real-valued function of $\mathbf{x}$, $W(\mathbf{x}) = W(-\mathbf{x})$, and $W(\mathbf{x})\in L^1\equiv L^1(R^3)$ (the space of integrable functions on R^3).

(iii) $v(\mathbf{x})$ is a random function of the form $v(\mathbf{x},\omega) = u(\mathbf{x},\omega)\mathrm{X}_G(\mathbf{x})$, where $u(\mathbf{x},\omega)$ is a (statistically) given real-valued homogeneous random function of $\mathbf{x}$, with zero average $\langle u(\mathbf{x})\rangle = 0$ and correlation coefficient $B(\mathbf{x}-\mathbf{y}) = \langle u(\mathbf{x})u(\mathbf{y})\rangle \equiv (u(\mathbf{x}),u(\mathbf{y}))$, so that $\langle v(\mathbf{x})\rangle = 0, \langle v(\mathbf{x})v(\mathbf{y})\rangle = B(\mathbf{x}-\mathbf{y})\mathbf{X}_G(\mathbf{x})\mathbf{X}_G(\mathbf{y})$. Therefore, $u(\mathbf{x})$ admits the spectral representation[2] $u(\mathbf{x}) = \int_{R^3}\exp(i\lambda\cdot\mathbf{x})d\Sigma(\lambda)$, where $\Sigma(\Delta)$ is a generalized orthogonal measure on (Borel) measurable sets $\Delta\subset R^3$, with values in $L^2(\Omega)$. Here, $\mathrm{X}_G(\mathbf{x})$ denotes a function of class $C_0^\infty(G)$ (i.e., a real-valued analytic function with compact support in G, $G\subset R^3$) which approximates (pointwise) the characteristic function of G and is otherwise arbitrary,[3] and $B(\mathbf{x}) = B(-\mathbf{x})$ is a given real-valued positive function of class $L^1\cap C^2(R^3)$. Technically, $u\in L^2(\Omega)\ \forall\mathbf{x}\in R^3, u\in C^2(R^3)$ for P-a.e. $\omega\in\Omega$, $u(\mathbf{x})\in L^1(\Omega\times R^3)$ and $u(\mathbf{x})u(\mathbf{y})\in L^1(\Omega\times R^3\times R^3)$.

(iv) Denoting by l a characteristic length of the region G where the potential V fluctuates randomly, defined, e.g., as $l^3 = \mathrm{vol}(G)$, and by $a_0^3 = \int_{R^3} B(\mathbf{x})[B(0)]^{-1}d\mathbf{x}$ the integral correlation scale a_0 of the fluctuations of $v(\mathbf{x})$, the inequality $\sqrt{a_0}\ll\sqrt{l}$ is fulfilled, i.e., the correlation scale is much smaller than the statistical range l of $v(\mathbf{x})$.

(v) The stochastic operator $A = L_0 - U - V$, where L_0 includes the Sommerfeld radiation condition, commutes with the operation of statistical averaging, in the sense that $\langle A\bar{\psi}\rangle = \langle A\rangle\bar{\psi}$ and $\langle L_0\psi\rangle = L_0\langle\psi\rangle$. This entails suitable hypotheses on $\nabla^2\psi$, to ensure uniform convergence of the integral $\int_\Omega\nabla^2\psi(\mathbf{x},\omega)dP$.

Observe also that the stochastic operator A is (formally) symmetric in $L^2(R^3)$ and satisfies the requirement of time-reversal invariance[4] (for P-a.e. $\omega\in\Omega$).

The analog of Eq. (1) for bound states (with local potential) has been investigated by P. Caldirola and his school (see Ref. 5) in order to give an alternative explanation of the well-known shift of the energy levels of hydrogenoid atoms ("Lamb-shift"). A functional-analytic study of the Schrödinger equation with nonlocal potential (in the deterministic case) may be found in a series of papers by G. Talenti *et al.* (see Ref. 6). The general subject of stochastic equations has been very thoroughly investigated recently[7-11]; of particular relevance are the results obtained by J. B. Keller and his school.[12-17] The use of nonlocal potentials is required in many problems, including the theory of nuclear matter and low-energy nucleon–nucleus scattering.[18-20]

2. RESULTS AND DISCUSSION

From Eqs. (1) and (3) we obtain

$$L_0\bar{\psi} + L_0\varphi = U\bar{\psi} + U\varphi + V\bar{\psi} + V\varphi. \tag{4}$$

We shall neglect, in a first approximation, the term $V\varphi$ in Eq. (4), assuming both v and φ to be very small perturbations; a precise evaluation of the error, however, will not be given here. Taking the average of Eq. (4) and subtracting them yields

$$L_0\bar{\psi} = U\bar{\psi}, \tag{5}$$

$$L_0\varphi = U\varphi + V\bar{\psi}. \tag{6}$$

The interchange in the order of the operations of sta-

tistical averaging and action by the operator A is justified by assumption (v).

Equation (5) is the usual Schrödinger equation for (local) potential scattering, whose asymptotic solution, under suitable assumptions for $U(\mathbf{x})$, is well known[4,18]:

$$\bar{\psi}_\infty(\mathbf{x}) = \exp(i\mathbf{k}_0\cdot\mathbf{x}) + f(\mathbf{k}_0,\mathbf{k})r^{-1}\exp(ikr), \quad (r = |\mathbf{x}|\to\infty). \tag{7}$$

Here, $\mathbf{k}_0$ is the wavenumber of the free incident particle $\mathbf{k} = (kr^{-1})\mathbf{x}$, $k = |\mathbf{k}| = |\mathbf{k}_0|$ (elastic scattering), and $f(\mathbf{k}_0,\mathbf{k})$ is an analytic function of k which describes the (deterministic) scattering.[4]

Denoting by M_0 the inverse operator of L_0, taking into account the Sommerfeld radiation condition,[18] Eq. (6) yields

$$\varphi = M_0U\varphi + M_0V\bar{\psi}, \tag{8}$$

where

$$M_0g = -(2m/\hbar^2)\int_{R^3}\exp(ik|\mathbf{x}-\mathbf{y}|)(4\pi|\mathbf{x}-\mathbf{y}|)^{-1}g(\mathbf{y})d\mathbf{y}.$$

In the Born approximation, by replacing $\bar{\psi}$ by $\bar{\psi}_0 = \exp(i\mathbf{k}_0\cdot\mathbf{x})$, Eq. (8) gives the following approximate value for $\varphi(\mathbf{x})$:

$$\varphi = M_0V\bar{\psi}_0, \tag{9}$$

which is independent of $U(\mathbf{x})$. Again, a precise evaluation of the error involved in the substitution of $\bar{\psi}$ by $\bar{\psi}_0$ will not be given here.

Denoting by F the Fourier transform in R^3, defined by

$$F[g](\boldsymbol{\lambda}) = \int_{R^3}\exp(-i\boldsymbol{\lambda}\cdot\mathbf{x})g(\mathbf{x})d\mathbf{x} \quad (\forall g\in L^1)$$

and by $\circ$ the convolution product in R^3, defined by

$$g_1\circ g_2 = g_2\circ g_1 = \int_{R^3}g_1(\mathbf{x}-\mathbf{y})g_2(\mathbf{y})d\mathbf{y},$$

we find

$$V\bar{\psi}_0 = v\bar{\psi}_0F[W](\mathbf{k}_0) + W\circ(v\bar{\psi}_0). \tag{10}$$

Since $V\bar{\psi}_0\in L^1\cap L^2(R^3)$ (for a.e. $\omega\in\Omega$), the asymptotic solution of (9) for $r\to\infty$ is

$$\varphi_\infty(\mathbf{x}) = \frac{2m}{\hbar^2}\frac{\exp(ikr)}{-4\pi r}F[V\bar{\psi}_0](\mathbf{k})$$

and, by an application of the convolution theorem for Fourier transforms,[3] we obtain

$$\begin{aligned}\varphi_\infty(\mathbf{x}) &= \frac{2m}{\hbar^2}\frac{\exp(ikr)}{-4\pi r}\{F[v\bar{\psi}_0](\mathbf{k})F[W](\mathbf{k}_0)\\ &\quad + F[v\bar{\psi}_0](\mathbf{k})F[W](\mathbf{k})\}\\ &= \frac{2m}{\hbar^2}\frac{\exp(ikr)}{-4\pi r}F[v](\mathbf{k}-\mathbf{k}_0)\{F[W](\mathbf{k}) + F[W](\mathbf{k}_0)\}.\end{aligned} \tag{11}$$

Thus, the asymptotic solution of (1) for $r\to\infty$ under the stated assumptions reads

$$\psi_\infty = \bar{\psi}_\infty + \varphi_\infty = \bar{\psi}_0 + [f(\mathbf{k}_0,\mathbf{k}) + f_s(\mathbf{k}_0,\mathbf{k})]\exp(ikr)/r, \tag{12}$$

where f_s is given by (11). The differential scattering cross section is then

$$\begin{aligned}\sigma(\mathbf{k}_0,\mathbf{k}) &= \langle|f(\mathbf{k}_0,\mathbf{k}) + f_s(\mathbf{k}_0,\mathbf{k})|^2\rangle\\ &= |f|^2 + \langle|f_s|^2\rangle = \sigma_d + \sigma_s,\end{aligned} \tag{13}$$

where the stochastic contribution $\sigma_s = \langle f_sf_s^*\rangle$ is found from (11) to be of the form

$$\begin{aligned}\sigma_s(\mathbf{k}_0,\mathbf{k}) &= r^2\langle\varphi_\infty\varphi_\infty^*\rangle\\ &= (4m^2/16\pi^2\hbar^4)\langle|F[v](\mathbf{k}-\mathbf{k}_0)|^2\rangle|F[W](\mathbf{k})\\ &\quad + F[W](\mathbf{k}_0)|^2.\end{aligned} \tag{14}$$

Taking assumptions (iii) and (iv) into account, we have

$$\begin{aligned}\langle|F[v](\mathbf{k}-\mathbf{k}_0)|^2\rangle &= \iint_{R^3}\exp[-i(\mathbf{k}-\mathbf{k}_0)\\ &\quad\cdot(\mathbf{x}-\mathbf{y})]\langle v(\mathbf{x})v(\mathbf{y})\rangle d\mathbf{x}d\mathbf{y}\\ &= \iint_{R^3}\exp[-i(\mathbf{k}-\mathbf{k}_0)\\ &\quad\cdot(\mathbf{x}-\mathbf{y})]B(\mathbf{x}-\mathbf{y})X_G(\mathbf{x})X_G(\mathbf{y})d\mathbf{x}d\mathbf{y}\\ &\cong \mathrm{vol}(G)F[B](\mathbf{k}-\mathbf{k}_0) = l^3\Phi(\mathbf{k}-\mathbf{k}_0),\end{aligned}$$

neglecting terms of the order $\sigma(\sqrt{a_0/l})$. Here, $\Phi(\boldsymbol{\lambda})$ denotes the spectrum[2] of the fluctuations of $u(\mathbf{x})$, i.e., the Fourier transform of $B(\mathbf{x})$, related to $\Sigma(\Delta)$ by $\langle|\Sigma(\Delta)|^2\rangle = \int_\Delta\Phi(\boldsymbol{\lambda})d\boldsymbol{\lambda}$ for every (Borel) measurable set $\Delta\subset R^3$.

Hence, the stochastic cross section reads

$$\sigma_s = (m^2l^3/4\pi^2\hbar^4)\Phi(\mathbf{k}-\mathbf{k}_0)|F[W](\mathbf{k}) + F[W](\mathbf{k}_0)|^2, \tag{15}$$

and is independent of $U(\mathbf{x})$. It is seen that, due to the nonlocal nature of V, σ_s depends not only on the difference $\mathbf{k}-\mathbf{k}_0$, but separately (and symmetrically) upon $\mathbf{k}$ and $\mathbf{k}_0$.

In the limit case of a local random potential $V = 2v\delta\circ$ [where $\delta(\mathbf{x})$ denotes, as usual, the Dirac distribution], we have $W(\mathbf{x}) = \delta(\mathbf{x})$, whence

$$\sigma_s = (m^2l^3/\pi^2\hbar^4)\Phi(\mathbf{k}-\mathbf{k}_0). \tag{16}$$

If the homogeneous random function $u(\mathbf{x})$ is also isotropic, then $B(\mathbf{x}) = B(|\mathbf{x}|)$, and we find

$$\Phi(\mathbf{k}-\mathbf{k}_0)\equiv\Phi(\xi) = 4\pi\int_0^\infty r^2B(r)[\xi r]^{-1}\sin(\xi r)\,dr, \tag{17}$$

where $\xi = |\mathbf{k}-\mathbf{k}_0|$. In the complex ξ plane, $\Phi(\xi)$ thus converges on the real ξ axis and is (possibly) a holomorphic function of ξ in a horizontal strip centered on the real axis. In the case of a Markovian correlation function,[2]

$$B(r) = q^2\exp[-2\pi^{1/3}a_0^{-1}r], \quad q^2 = \langle u^2(\mathbf{x})\rangle, \tag{18}$$

$\Phi(\xi)$ appears to be holomorphic in the strip $|\mathrm{Im}\xi| < 2\pi^{1/3}a_0^{-1}$ [see Eq. (21)]. However, taking assumptions (iii) and (iv) into account, we see that, in the same order of approximation of Eqs. (9) and (15), σ_s must be holomorphic on the whole complex ξ plane.

More accurate insight into the analytic properties of the stochastic scattering amplitude $f_s(\mathbf{k}_0,\mathbf{k}_0)$ (for $\mathbf{k} = \mathbf{k}_0$) as

a function of E may be gained by replacing the approximate equation (9) by the formula $\varphi = M_0 V\bar{\psi}$ (which is exact to the first order in φ). We obtain then the following expression for $f_s(\mathbf{k}_0, \mathbf{k}_0)$:

$$f_s(\mathbf{k}_0, \mathbf{k}_0) = -(m/2\pi\hbar^2)F[V\bar{\psi}](\mathbf{k}_0) = -(m/2\pi\hbar^2)\{F[vW\circ\bar{\psi}](\mathbf{k}_0) + F[W](\mathbf{k}_0)F[v\bar{\psi}](\mathbf{k}_0)\}, \tag{19}$$

where $\bar{\psi}$ depends on E, being a solution of Eq. (5). Thus, in the case of a local potential, writing, as usual, the energy E as a complex variable, with $E = [\hbar^2(2m)^{-1}]k^2$, $f_s(\mathbf{k}_0, \mathbf{k}_0)$ is (for a.e. $\omega \in \Omega$) a holomorphic function of E on the whole physical sheet $\mathrm{Im}k \geq 0$ of the Riemann surface of the energy,[4] with the exception of the points where $\bar{\psi}$ becomes infinite. These poles, where $f_s(E)$ is singular, are located on the real semiaxis $E < 0$ and correspond to the discrete unperturbed energy levels, i.e., to the bound states of the potential $U(\mathbf{x})$ (eigenvalues of the operator $L_0 - U$).[4,18]

In the case of a nonlocal potential, the first term on the right-hand side of (19) is still holomorphic for $\mathrm{Im}k \geq 0$ while the second term is holomorphic in a horizontal strip of width β_0, centered on the real k axis, corresponding to the analyticity domain of $F[W](\mathbf{k}_0) = \int_{R^3} \exp(-ikz)W(x,y,z)\,dxdydz$. Thus, $f_s(\mathbf{k} = \mathbf{k}_0)$ is, for a.e, $\omega \in \Omega$, holomorphic in the interior of a parabolic region, enclosing (symmetrically) the real semiaxis $E \geq 0$ and additional singularities (besides the eigenvalues of $L_0 - U$) may appear on the real negative E axis outside the parabola, i.e., for $\mathrm{Re}E < -\beta_0^2\hbar/2m$. The value of β_0 depends upon the regularity properties of $W(\mathbf{x})$. If $\beta_0 = 0$, the convergence region of f_s shrinks to the real k axis $\mathrm{Im}k = 0$, i.e., to the (cut along the) real semiaxis $E > 0$,[4,19,20] since $F[W](\mathbf{k}_0)$ is then a bounded and continuous (but not necessarily analytic) function of real k.

The characteristic length l appearing in Eqs. (15) and (16) depends on the specific problem under consideration; two simple examples will be considered in the next section.

3. EXAMPLES

Consider first a random potential trough (or barrier) with spherical symmetry[1] $W(\mathbf{x}) = \delta(\mathbf{x})$ and $v(\mathbf{x}) = v_0 H(l - r)$, where $H(r)$ is the Heaviside step function and v_0 is a real random variable with zero average and given variance $q^2 = \langle v_0^2 \rangle$. It follows $\langle v(\mathbf{x})v(\mathbf{y})\rangle = q^2 H(l - |\mathbf{x}|)H(l - |\mathbf{y}|)$, whence,

$$\sigma_s = (16m^2q^2/\hbar^4\xi^4)\,|\xi^{-1}\sin(l\xi) - l\cos(l\xi)|^2. \tag{20}$$

σ_s thus coincides formally with the (deterministic) cross-section in the Born approximation, and exhibits likewise the Gibbs oscillatory phenomenon due to the truncation in $v(\mathbf{x})$ [see Assumption (iii), which is not satisfied here].

Consider next the case of a Markovian correlation function (18); from Eq. (17) we find

$$\Phi(\xi) = \pi^{2/3}q^2a_0^3\left[1 + \frac{a_0^2}{4\pi^{2/3}}\xi^2\right]^{-2}. \tag{21}$$

Choosing a system of spherical polar coordinates with polar axis parallel to $\mathbf{k}_0$, and denoting θ the colatitude (angle of scattering), we have $\xi = |\mathbf{k} - \mathbf{k}_0| = 2k\sin(\theta/2)$,[1] and Eq. (16) for a local potential gives

$$\sigma_s = (m^2q^2a_0^3/\hbar^4\pi^{4/3})l^3[1 + (k^2a_0^2/\pi^{2/3})\sin^2(\theta/2)]^{-2}, \quad 0 \leq \theta \leq \pi. \tag{22}$$

σ_s is thus a monotone decreasing function of θ, and, if the correlation scale a_0 satisfies the inequality $ka_0 \ll 1$, σ_s is approximately constant (isotropic scattering[1]).

If $U(\mathbf{x}) \equiv 0$, we have $f(\mathbf{k}_0, \mathbf{k}) = 0$ while $\sigma = \sigma_s > 0$ and, as shown by Eq. (20), the expression of σ_s may happen to coincide formally with the nonrandom case ($V = 0$, $U \neq 0$). In particular, the physical interpretation of Eq. (20) is the following: a potential trough (or barrier) which oscillates randomly about zero exhibits the same scattering behavior of a nonrandom potential trough (barrier) with the same (average) depth.

4. FINAL REMARKS

The case of a stochastic operator V with average value $\bar{V}$ different from zero can be reduced to the previous one by replacing U by $U + \bar{V}$ and V by $V - \bar{V}$ in the preceding formulas. Therefore, if $\bar{V} \neq 0$ only the terms involving the operator U, i.e., only the average wavefunction $\bar{\psi}$, will be modified, since in the first approximation $\bar{\psi}(\mathbf{x})$ will satisfy the equation

$$L_0\bar{\psi} = U\bar{\psi} + \bar{V}\bar{\psi}. \tag{23}$$

Let us restrict ourselves to the case of a local potential V, represented by the operator of multiplication by a random function $V(\mathbf{x})$. $\bar{V}$ is then the operator of multiplication by the real-valued function $\bar{V}(\mathbf{x})$, which gives the average value of the stochastic potential V, and must be specified on the basis of dynamical considerations.

Assuming the random fluctuations of the potential to be originated by statistical fluctuations $d\mathbf{x}$ in the position of the particle, and, expanding the potential in a Taylor series, we have[5]

$$U(\mathbf{x}) + V(\mathbf{x}) \equiv U(\mathbf{x} + d\mathbf{x}) = U(\mathbf{x}) + (d\mathbf{x})\cdot\mathrm{grad}U + \frac{1}{2}\sum_{i,j=1}^{3}\left(\frac{\partial^2 U}{\partial x_i \partial x_j}\right)dx_i dx_j + \cdots. \tag{24}$$

Taking the average of Eq. (24), assuming $\langle d\mathbf{x}\rangle = 0$ and $\langle dx_i dx_j\rangle = \frac{1}{3}\langle |dx|^2\rangle\,\delta_{i,j}$ due to symmetry, and neglecting terms of higher order in (24) yields

$$\langle V(\mathbf{x})\rangle \equiv \bar{V}(\mathbf{x}) = \tfrac{1}{6}\langle |d\mathbf{x}|^2\rangle\nabla^2 U(\mathbf{x}). \tag{25}$$

In the case of a screened Coulomb field $U(\mathbf{x}) = -e^2r^{-1}\exp(-\alpha r)$, we have $\nabla^2 U(\mathbf{x}) = 4\pi e^2\delta(\mathbf{x}) + \alpha^2 U(\mathbf{x})$, where e is the charge unit and α is a positive constant. The expression of σ_s contains, then, an additional perturbation term of the form

$$(m^2/4\pi^2\hbar^4)\,|\int_{R^3}\bar{\psi}_0\bar{V}(\mathbf{x})\bar{\psi}_1^*d\mathbf{x}|^2, \tag{26}$$

where $\bar{\psi}_1 = \exp(i\mathbf{k}\cdot\mathbf{x})$. In the limit $\alpha \to 0$, taking Eq. (25) into account, Eq. (26) reduces to $[(1/9r_B^2)[\langle |d\mathbf{x}|^2\rangle)^2]$, where $r_B = \hbar^2/me^2$ is the Bohr radius.[4] Thus, in the case of a (weakly) screened Coulomb potential with nonvanishing average value the cross-section is increased by a constant term, corresponding to an additional isotropic scattering.

In the case of a complex atom of atomic number Z, assuming $U(\mathbf{x})$ to satisfy the Thomas–Fermi equation, we find[4]

$$\overline{V}(\mathbf{x}) = \tfrac{1}{6}\langle |d\mathbf{x}|^2\rangle\{-4\pi e^2 Z\delta(\mathbf{x}) + (8\sqrt{2}/3\pi e)[U(\mathbf{x})/r_B]^{3/2}\}, \tag{27}$$

where $|\mathbf{x}|U(\mathbf{x}) \to 0$ for $|\mathbf{x}| \to \infty$, $|\mathbf{x}|U(\mathbf{x}) \to Ze^2$ for $\mathbf{x} \to 0$.[4] The additional perturbation term in the expression of σ_s is found from Eqs. (26) and (27) to be of the form

$$(1/9r_B^2)(\langle |d\mathbf{x}|^2\rangle)^2 |-Z + (2\sqrt{2}/3\pi^2)(e^2 r_B)^{-3/2} \times F[U^{3/2}](\mathbf{k}-\mathbf{k}_0)|^2, \tag{28}$$

while the terms involving $\varphi(\mathbf{x})$ remain unaltered, provided V is replaced by $V - \overline{V}$, as explained above.

The value of $\langle |d\mathbf{x}|^2\rangle$ must still be specified in the preceding formulas. Following Caldirola's semiclassic reasoning for an s electron of hydrogenoid atom yields[5]

$$\langle |d\mathbf{x}|^2\rangle = (e^2\hbar/3\pi m^2 c^3)\log(\nu_1/\nu_2), \tag{29}$$

where c is the light speed in vacuum, and $\nu_2 \ll \nu_1$ are limit frequencies of the "electromagnetic fluctuation field", to be determined in a heuristic way (in Ref. 5, $\nu_1/\nu_2 \simeq 10^{14}$).

*Research developed in the frame of the activity of the GNFM of the CNR.

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On the inverse problem for a hyperbolic dispersive partial differential equation. II

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In a previous paper the inverse problem for a dispersive hyperbolic partial differential equation was shown to be reducible to a system of two coupled integral equations involving the kernels of the scattering operators. Here the uniqueness question is considered. The conditions on the scattering kernel to insure uniqueness of the solution of the system of integral equations are developed.

In the previous paper,[1] which we will refer to as Paper I the inverse problem related to the partial differential equation

$$u_{xx} - u_{tt} + A(x)u_x + B(x)u_t + C(x)u = 0,$$

where the coefficients vanish outside the domain $0 < x < l$, was considered. For an incident wave $u_+^i(x - t)$ propagating in the direction of the positive x axis, a reflected wave $u_+^r(x + t)$ and a transmitted wave $u_+^t(x - t)$ are generated which can be expressed in terms of the incident wave by back and forward scattering operators. A similar result holds for an incident wave $u_-^i(x + t)$ propagating in the direction of the negative x axis. It was shown that the inverse problem, namely the determination of the coefficients A, B and C from the kernels of the scattering operators, reduced to the problem of solving the two coupled integral equations, (24a) and (25a) of Paper I. The question of uniqueness was only partially answered. Here, we consider the question of uniqueness further, and will determine conditions on the scattering kernels for which the following homogeneous system of integral equations corresponding to Eqs. (24a) and (25a) of Paper I, has only the trivial solution

$$\begin{aligned} \varphi(t) &= -\int_{-\mu}^{\mu} S_+(y,t)\psi(y)dy, \qquad \mu \le t < 2l-\mu, \\ \psi(t) &= -G(l)\int_{\mu}^{2l-\mu} S_-(y,t)\varphi(y)dy, \qquad -\mu < t < \mu. \end{aligned} \tag{1}$$

For convenience we have replaced the parameter x which appears in the corresponding nonhomogeneous integral equations in Paper I by the parameter μ.

To determine conditions for which system (1) has only the trivial solution, we will relate the solutions of the corresponding adjoint system of integral equations to the solutions of an initial-boundary value problem of the partial differential equation. Before doing so, we begin with some general considerations.

Consider the Cauchy problem

$$\begin{aligned} &u_{xx} - u_{tt} + A(x)u_x + B(x)u_t + C(x)u = 0, \\ &u(x,t_0) = f(x - t_0) + g(x + t_0), \\ &u_t(x,t_0) = -f'(x - t_0) + g'(x + t_0), \end{aligned} \tag{2}$$

where A, B, C are C^1 functions with support in $[0, l]$ and f, g are continuous, piecewise C^2 (written $C[C^2$ piecewise]) functions. Using the method of successive approximations,[2] it can be shown that this problem is well posed in the appropriate class of $C[C^2$ piecewise] functions. For example, if $f'(s), g'(s)$ are discontinuous at $s = \alpha$, $s = \beta$ respectively, then the solution u will be C^2 except across the lines $x - t = \alpha, x + t = \beta$ where it is continuous. In what follows we shall omit reference to the regions on which a solution is C^2 and assume that the obvious $C[C^2$ piecewise] class of functions is chosen.

This result enables us to generalize the lemma in Paper I. Specifically, that lemma remains valid under the weaker assumption that the Cauchy data is $C[C^2$ piecewise].

Lemma 1: Suppose u is the $C[C^2$ piecewise] solution of (2) subject to initial conditions at $t = -l$,

$$\begin{aligned} u(x,-l) &= f(x + l) + g(x - 3l + 2\mu), \\ u_t(x,-l) &= -f'(x + l) + g'(x - 3l + 2\mu), \end{aligned}$$

where $f(s)$ and $g(s)$ are arbitrary continuous functions which are C^2 on their supports $-(2l - 2\mu) \le s \le 0$ and $0 \le s \le 2\mu$, respectively, and $0 < \mu < l$. If u also satisfies the boundary conditions

$$\begin{aligned} u(0,t) &= 0, \qquad 2l - 2\mu < t < 2l, \\ u(l,t) &= 0, \qquad l < t < 3l - 2\mu, \end{aligned}$$

then $u \equiv 0$.

Proof: The initial conditions correspond to the superposition of two incident waves of the form

$$\begin{aligned} u_+^i(x - t) &= f(x - t), \qquad x < 0 \\ u_-^i(x + t - 2l + 2\mu) &= g(x + t - 2l + 2\mu), \qquad x > l. \end{aligned}$$

Hence, for $x < 0, t > 2l - 2\mu$ we have that u is a function of $x + t$ only. The first boundary condition then implies that $u = 0$ in the strip bounded by $x + t = 2l, x + t = 2l - 2\mu$ and $x = 0$. Similarly, $u = 0$ in the strip bounded by $x - t = 0, x - t = 2\mu - 2l$ and $x = l$.

It now follows that $u_x(0,t) = 0$ for $2l - 2\mu < t < 2l$ and $u_x(l,t) = 0$ for $l < t < 3l - 2\mu$. Thus, $u = 0$ in the triangles T_1 and T_2, where T_1 is bounded by $x + t = 2l$, $x - t = 2\mu - 2l$ and $x = 0$ and T_2 is bounded by $x + t = 2l$, $x - t = 2\mu - 2l$ and $x = l$.

Using the fact that the solution of a characteristic initial value problem[2] is unique, we get that $u = 0$ in the rectangle R bounded by $T_1, T_2, x + t = 2l - 2\mu$ and $x - t = 0$. We also know that $u = 0$ in the triangle T_3 bounded by $x - t = 0, x + t = 2l - 2\mu$ and $t = -l$. Then $u = 0$ in the triangles bounded by R, T_3 and the lines $x = 0, x = l$, and so $u \equiv 0$.

We now consider the system of integral equations adjoint to system (1),

$$\varphi(t) = -G(l)\int_{-\mu}^{\mu} R_-(t+s)[\psi(s) + \int_{-\mu}^{s} L_-(s-y)\psi(y)dy]ds, \quad \mu < t < 2l-\mu,$$
$$\psi(t) = -\int_{\mu}^{2l-\mu} R_+(t+s)[\varphi(s) + \int_{s}^{2l-\mu} L_+(s-y)\varphi(y)dy]ds, \quad -\mu < t < \mu. \tag{3}$$

Lemma 2: The only solution φ, ψ of the system of integral equations (3) where φ is C^2 on $[\mu, 2l-u]$ and ψ is C^2 on $[-\mu, \mu]$ and which satisfy the conditions $\varphi(2l-\mu) = 0$, $\psi(-\mu) = 0$, $p(\mu) = 0$, $q(\mu) = 0$ where

$$p(t) = \varphi(t) + \int_{t}^{2l-\mu} L_+(t-y)\varphi(y)dy,$$
$$q(t) = \psi(t) + \int_{-\mu}^{t} L_-(t-y)\psi(y)dy \tag{4}$$

is the trivial solution.

Proof: On employing the scattering operators given in Paper I, we can relate the above set of integral equations to the solution of the differential equation and associated boundary and initial conditions as described by Lemma 1.

In the half-space $x \le 0$, the incident wave $u_+^i(x-t)$ generates a reflected wave $u_+^r(x+t)$ and a transmitted wave $u_+^t(x-t)$ in the half-space $x \ge l$. They are related as follows

$$u_+^r(\xi) = \int_{-\xi}^{0} R_+(\xi+s)u_+^i(s)ds, \quad \xi > 0$$
$$u_+^i(\eta) = \exp\tfrac{1}{2}\int_0^l (A-B)ds\{u_+^t(\eta) + \int_{\eta}^{0} L_+(\eta-s)u_+^t(s)ds\}, \quad \eta < 0$$

with $u_+^r(\xi) = 0$, $u_+^i(\eta) = 0$ for $\xi < 0$, $\eta > 0$, respectively.

Similarly, in the half-space $x \ge l$, the incident wave $u_-^i(x+t-2l+2\mu)$ generates the reflected wave $u_-^r(x-t+2l-2\mu)$; and in the half-space $x \le 0$, a transmitted wave $u_-^t(x+t-2l+2\mu)$. These are related as follows:

$$u_-^r(\eta) = \int_0^{2l-\eta} R_-(s+\eta)u_-^i(s)ds, \quad \eta \le 2l,$$
$$u_-^i(\xi) = \exp-\tfrac{1}{2}\int_0^l (A+B)ds\{u_-^t(\xi) + \int_0^{\xi} L_-(\xi-s)u_-^t(s)ds\}, \quad \xi \ge 0,$$

where $u_-^i(\xi) = 0$ for $\xi < 0$.

To agree with the initial conditions given in Lemma 1, namely

$$u(x,t) = u_+^i(x-t) + u_-^i(x+t-2l+2\mu), \quad t \le -l,$$

where $u_+^i(s)$ and $u_-^i(s)$ are C^2 functions of s on their respective supports $-(2l-2\mu) \le s \le 0$ and $0 \le s \le 2\mu$, the definition of $\varphi(s)$ and $\psi(s)$ will have to be extended outside their respective domains $\mu \le s \le 2l-\mu$ and $-\mu \le s \le \mu$ so that they still remain $C[C^2$ piecewise]. This can be achieved by defining

$$\varphi(s) \equiv 0 \quad \text{for } s > 2l-\mu$$

and

$$p(s) \equiv \varphi(s) + \int_{s}^{2l-\mu} L_+(s-y)\varphi(y)dy = 0 \quad \text{for } s < \mu.$$

This will place no further restriction on $\varphi(s)$ in the domain $\mu \le s \le 2l-2\mu$ other then the conditions

$$\varphi(2l-\mu) = p(\mu) = 0,$$

as stated in the lemma. In a similar manner, $\psi(s)$ may be extended outside its domain.

The boundary conditions stated in Lemma 1 now become

$$u_-^t(t-2l+2\mu) + u_+^t(t) = 0, \quad 2l-2\mu \le t \le 2l,$$
$$u_+^t(l-t) + u_-^r(-t+3l-2\mu) = 0, \quad l \le t \le 3l-2\mu,$$

yielding

$$\psi(\tau) = -\int_{\mu}^{2l-\mu} R_+(\tau+s)p(s)ds, \quad -\mu \le \tau \le \mu,$$
$$\varphi(\tau) = -G(l)\int_{-\mu}^{\mu} R_-(\tau+s)q(s)ds, \quad \mu \le \tau \le 2l-\mu.$$

Then the system of integral equations and conditions stated in this lemma are equivalent to the initial-boundary value problem given in Lemma 1, and the result follows.

A different formulation of Lemma 2 will be more useful. Suppose φ, ψ is a solution of (3) where $\varphi \in L^2(\mu, 2l-\mu)$, $\psi \in L^2(-\mu, \mu)$. Since R_+, R_-, L_- are C^2 on $[0, 2l]$ and L_+ is C^2 on $[-2l, 0]$, it follows that φ, ψ are C^2 on $[\mu, 2l-\mu]$ and $[-\mu, \mu]$ respectively.

For $i = 1, 2$ let

$$\theta_i(t) = \tilde{\theta}_i(t) + \int_{\mu}^{t} L_+(y-t)\tilde{\theta}_i(y)dy, \quad \mu < t < 2l-\mu,$$
$$\chi_i(t) = \tilde{\chi}_i(t) + \int_{t}^{\mu} L_-(y-t)\tilde{\chi}_i(y)dy, \quad -\mu < t < \mu,$$

where

$$\tilde{\theta}_1(t) = 1, \quad \tilde{\chi}_1(t) = 1,$$
$$\tilde{\theta}_2(t) = \int_{\mu}^{t} R_+(y-\mu)dy, \quad \tilde{\chi}_2(t) = \int_{\mu}^{t} R_-(y+2l-\mu)dy.$$

Let N_1 be the subspace of $L^2(\mu, 2l-\mu)$ spanned by θ_1, θ_2 and let N_2 be the subspace of $L^2(-\mu, \mu)$ spanned by χ_1, χ_2. Finally, let $N_1^{\perp}, N_2^{\perp}$ be the corresponding orthogonal compliments where the inner products are

$$(\theta, \theta_i) = \int_{\mu}^{2l-\mu} \theta\theta_i dt, \quad (\chi, \chi_i) = \int_{-\mu}^{\mu} \chi\chi_i dt,$$

respectively. Then we have

Lemma 3: The only L^2 solution φ, ψ of the system of integral equations (3) such that $\varphi \in N_1^{\perp}, \psi \in N_2^{\perp}$ is the trivial solution.

Proof: Suppose φ_0, ψ_0 satisfy the above hypotheses. Set

$$\varphi_1(t) = \int_{2l-\mu}^{t} \varphi_0(y)dy, \quad \mu < t < 2l-\mu,$$
$$\psi_1(t) = \int_{-\mu}^{t} \psi_0(y)dy, \quad -\mu < t < \mu$$

and for $i = 0, 1$ let $p_i(t), q_i(t)$ be the expressions given in (4) with φ_i, ψ_i in place of φ, ψ. The system (3) now becomes

$$\varphi_0(t) = -G(l)\int_{-\mu}^{\mu} R_-(t+s)q_0(s)ds, \quad \mu < t < 2l-\mu, \tag{5}$$

$$\psi_0(t) = -\int_{\mu}^{2l-\mu} R_+(t+s)p_0(s)ds, \quad -\mu < t < \mu. \tag{6}$$

Integrating (5) from $2l - \mu$ to t, we get

$$\varphi_1(t) = G(l) \int_{-\mu}^{\mu} R_-(t+s)q_1(s)ds,$$

where we have used the fact that $\psi_0 \in N_2^{\perp}$. Integration of (6) from $-\mu$ to t yields

$$\psi_1(t) = \int_{-\mu}^{\mu} R_+(t+s)p_1(s)ds$$

by virtue of the fact that $\varphi_0 \in N_1^{\perp}$. Now φ_1, ψ_1 satisfy the hypotheses of Lemma 2, so $\varphi_1 \equiv 0, \psi_1 \equiv 0$ and the lemma is proven.

Our main result follows from the alternative theorem.

Theorem: If none of the functions $\theta_1, \theta_2, \chi_1, \chi_2$ provide a solution of the system (3), then the only L^2 solution of the homogeneous system (1) is the trivial solution.

Hence, we have given conditions for the uniqueness of the inverse scattering problem given in Paper I. Note that we required that the coefficients A, B, C of the partial differential equation to be C^1.

ACKNOWLEDGMENT

This research was supported by National Science Foundation under Grant GP-22583.

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The evaluation of lattice sums. I. Analytic procedures

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Procedures are given for summing series of the form $\Sigma a_{ijk\ldots}(i^2+j^2+k^2+\cdots)^{-s}$ and used to evaluate a number of planar lattice sums in terms of the zeta and related functions.

I. INTRODUCTION

In calculations of the physical properties of crystal surfaces, one often requires numerical values for sums of the form

$$S = \sum_{m,n=1}^{\infty} f(m,n), \tag{1}$$

where most frequently $f(m,n)$ is the reciprocal of some power of a linear or quadratic expression. In the latter case, the sums have been investigated intensively and several methods are available for approximating them.[1] It has apparently escaped notice, however, that when $f(m,n)$ is a "symmetric quadratic form", S can often be expressed in terms of well-known, tabulated functions. There is some suggestive work by Emersleben[2] who considered the three dimensional case in terms of the Epstein zeta function, but his procedure merely amounts to an extension of Ewald's method.[3] The one result which exists in the literature,

$$\sum_{m,n=1}^{\infty} (m^2+n^2)^{-s} = \zeta(s)\beta(s) - \zeta(2s), \tag{2}$$

which is apparently due to Hardy,[4] who used number-theoretic considerations, is fairly typical of those we shall derive. Here $\zeta(s)$ is the well-known Riemann zeta function and

$$\beta(s) = \sum_{n=0}^{\infty} (-1)^n (2n+1)^{-s}, \tag{3}$$

has also been tabulated.[5] Since this function, which has apparently not been studied in detail previously, will play an important role in our analysis, its salient properties are presented in an appendix.

II. CALCULATION

The method we shall use is undoubtedly well known and is quite useful for the summation of multiple series where the summand contains a linear combination of expressions, each of which involves only one variable. Below we shall use the following notation. The variables of summation k and l are to run over all positive odd integers, the variables p and q are to run over all positive even integers, and m and n are to run over all positive integers. To introduce the technique, we consider the simple example

$$S = \sum_{k,l} (-1)^{(k-1)/2}(ak+l)^{-s}, \qquad s>0. \tag{4}$$

By using the identity

$$\Gamma(s)b^{-s} = \int_0^{\infty} x^{s-1}e^{-bx}dx \equiv M_s\{e^{-bx}\}, \tag{5}$$

where M_s denotes the Mellin transform,[6] we obtain

$$\Gamma(s)S = \int_0^{\infty} x^{s-1}\sum_{k,l}(-1)^{(k-1)/2}\exp[-(ak+l)x]dx = M_s\{\operatorname{sech}x\ \operatorname{csch}ax\}, \tag{6}$$

whence we have

$$S = 2^{-s}\{\Phi[-1,s,\tfrac{1}{2}(1+a)] + \Phi[-1,s,\tfrac{1}{2}(1-a)]\}, \tag{7}$$

where Φ denotes the Lerch–Hurwitz zeta function.[7] Here and in succeeding applications of this procedure, the interchange of the sum and the integral is justified by the absolute convergence of the former.

Consider now the five sums listed in Table I. All others of this general form can be obtained from these by elementary means. We first note the following basic identities from the theory of theta functions[8]:

$$\sum_m e^{-m^2x} = \tfrac{1}{2}[\theta_3(0\,|\,ix/\pi) - 1], \tag{8a}$$

$$\sum_m (-1)^{m-1}e^{-m^2x} = \tfrac{1}{2}[1-\theta_4(0\,|\,ix/\pi)], \tag{8b}$$

$$\sum_k e^{-k^2x} = \tfrac{1}{2}\theta_2(0\,|\,4ix/\pi), \tag{8c}$$

$$\sum_p e^{-p^2x} = \tfrac{1}{2}[\theta_3(0\,|\,4ix/\pi) - 1]. \tag{8d}$$

Next, by using (5), we have

$$\Gamma(s)S_1 = \tfrac{1}{4}M_s\{[\theta_3(0\,|\,ix/\pi) - 1]^2\}, \tag{9a}$$

$$\Gamma(s)S_2 = \tfrac{1}{4}M_s\{[1-\theta_4(0\,|\,ix/\pi)]^2\}, \tag{9b}$$

$$\Gamma(s)S_3 = \tfrac{1}{4}M_s\{[1-\theta_4(0\,|\,ix/\pi)][\theta_3(0\,|\,ix/\pi) - 1]\}, \tag{9c}$$

$$\Gamma(s)S_4 = \tfrac{1}{4}M_s\{\theta_2^2(0\,|\,4ix/\pi)\}. \tag{9d}$$

We postpone the evaluation of S_5 which requires a little further ground work.

To complete the derivation, we need the Mellin transforms of squares and products of theta functions. Since these have apparently not been studied before, we shall devote some space to working them out. In the following, the symbol $\cdot\sim\cdot$ is used to denote the relation of a func-

TABLE I.

Sum	$f(m,n)$	Value
S_1	$(m^2+n^2)^{-s}$	$\zeta(s)\beta(s) - \zeta(2s)$
S_2	$(-1)^{m+n}(m^2+n^2)^{-s}$	$(1-2^{1-2s})\zeta(2s) - (1-2^{1-2s})\beta(s)\zeta(s)$
S_3	$(-1)^{n-1}(m^2+n^2)^{-s}$	$2^{-s}[2^{-s}\zeta(2s) + (1-2^{1-s})\beta(s)\zeta(s)]$
S_4	$(k^2+l^2)^{-s}$	$2^{-s}(1-2^{-s})\beta(s)\zeta(s)$
S_5	$(m^2+p^2)^{-s}$	$\tfrac{1}{2}(1-2^{-s}+2^{1-2s})\zeta(s)\beta(s) - \tfrac{1}{2}(1+2^{-2s})\zeta(2s)$

tion to its Mellin transform. The following pairs follow immediately from Eqs. (5) and (8):

$$\tfrac{1}{2}[\theta_3(0|ix/\pi)-1] \cdot\sim\cdot \Gamma(s)\zeta(2s), \quad \mathrm{Re}\, s > \tfrac{1}{2}, \tag{10a}$$

$$\tfrac{1}{2}[1-\theta_4(0|ix/\pi)] \cdot\sim\cdot (1-2^{1-2s})\Gamma(s)\zeta(2s), \quad \mathrm{Re}\, s > 0, \tag{10b}$$

$$\tfrac{1}{2}\theta_2(0|4ix/\pi) \cdot\sim\cdot (1-2^{-2s})\zeta(2s), \quad \mathrm{Re}\, s > \tfrac{1}{2}, \tag{10c}$$

where the elementary identities

$$\begin{aligned}(1-2^{1-s})\zeta(s) &= 1^{-s}-2^{-s}+3^{-s}-\cdots,\\ (1-2^{-s})\zeta(s) &= 1^{-s}+3^{-s}+5^{-s}+\cdots.\end{aligned} \tag{11}$$

have been used.

We next note several remarkable identities discovered by Jacobi[9]

$$2K/\pi = 1+4\sum_k (-1)^{(p-1)/2} q^l (1-q^l)^{-1} \tag{12a}$$

$$2kK/\pi = 4q^{1/2}\sum_n q^{n-1}(1+q^{2n-1})^{-1}, \tag{12b}$$

$$2k'K/\pi = 1-4\sum_l (-1)^{(p-1)/2} q^l (1+q^l)^{-1}, \tag{12c}$$

where K denotes the complete elliptic integral of the first kind of modulus k, $k' = (1-k^2)^{1/2}$ and $q = \exp(-K(k')/\pi K)$. These are obtained by differentiating the Fourier series for the elliptic modular functions[10] and setting $x = 0$.

From the identities[11]

$$\theta_3^2(0|t) = 2K/\pi, \tag{13a}$$

$$\theta_2^2(0|t) = 2kK/\pi, \tag{13b}$$

$$\theta_4^2(0|t) = 2k'K/\pi, \tag{13c}$$

where $q = \exp(i\pi t)$, we now have

$$\tfrac{1}{4}[\theta_3^2(0|ix/\pi)-1] = \sum_l (-1)^{(l-1)/2}[e^{lx}-1]^{-1}, \tag{14a}$$

$$\tfrac{1}{4}[1-\theta_4^2(0|ix/\pi)] = \sum_l (-1)^{(l-1)/2}[e^{lx}+1]^{-1}, \tag{14b}$$

$$\tfrac{1}{4}\theta_2^2(0|4ix/\pi) = \sum_l [e^{2lx}+e^{-2lx}]^{-1}. \tag{14c}$$

Next we expand the summands in (14) as geometric series in e^{-lx}. The Mellin transform of the quantities on the right in (14) are obtained by integrating term by term and by combining the expressions so obtained with (10). We find

$$\tfrac{1}{4}[\theta_3(0|ix/\pi)-1]^2 \cdot\sim\cdot \Gamma(s)[\beta(s)\zeta(s)-\zeta(2s)], \quad \mathrm{Re}\, s > 1, \tag{15a}$$

$$\tfrac{1}{4}[1-\theta_4(0|ix/\pi)]^2 \cdot\sim\cdot \Gamma(s)[\zeta(2s)(1-2^{1-2s}) - \beta(s)\zeta(s)(1-2^{1-2s})], \quad \mathrm{Re}\, s > 0, \tag{15b}$$

$$\tfrac{1}{4}\theta_2^2(0|4ix/\pi) \cdot\sim\cdot 2^{-s}(1-2^{-s})\Gamma(s)\beta(s)\zeta(s), \quad \mathrm{Re}\, s > 1. \tag{15c}$$

We still require the Mellin transforms of products of pairs of theta functions. By using the procedure by which Landen's transformation can be derived,[12] we find

$$\theta_2(0|2t)\theta_3(0|2t) = \tfrac{1}{2}\theta_2^2(0|t), \tag{16a}$$

$$\theta_3(0|t)\theta_4(0|t) = \theta_4^2(0|2t), \tag{16b}$$

and thus from (16b) and (10) we have

$$\tfrac{1}{4}[\theta_3(0|ix/\pi)-1][1-\theta_4(0|ix/\pi)] \cdot\sim\cdot 2^{-s}\Gamma(s) \times [2^{-s}\zeta(2s)+(1-2^{1-s})\beta(s)\zeta(s)]. \tag{17}$$

Comparison of (15), (17) with (9) gives the results shown in Table I. To obtain S_5, we make use of (16a) and find

$$\theta_2(0|8ix/\pi)\theta_3(0|8ix/\pi) \cdot\sim\cdot 2^{1-s}(1-2^{-s})\Gamma(s)\beta(s)\zeta(s), \tag{18}$$

whence we see that

$$\sum_l (2l)^{-2s} + 2\sum_{l,m} (2l^2+8m^2)^{-s} = 2^{1-s}(1-2^{-s})\beta(s)\zeta(s), \tag{19}$$

from which the expression given for S_5 is an immediate consequence.

Our discussion has been limited to equilateral lattices. The same procedure can be used for other planar lattices to represent the sums as Mellin transforms of products of theta functions; but, except in special cases, there are no known simple identities analogous to those in Eq. (12) which would lead to their evaluation. These representations can serve as the starting points for approximation schemes, however, of which Ewald's technique[3] is a disguised example.

Finally, we wish to illustrate how our results might be used to investigate more complicated lattice sums. Consider

$$S = \sum_{m,n} F(m^2+n^2). \tag{20}$$

Let $f(t)$ be the inverse Laplace transform of $F(u)$ and $\phi(s)$ be the Mellin transform of $f(t)$. Then

$$\begin{aligned} S &= \int_0^\infty dt\, f(t) \sum_{m,n} \exp[-(m^2+n^2)t]\\ &= \tfrac{1}{4}\int_0^\infty dt\, f(t)\left[\theta_3\left(0|\frac{it}{\pi}\right)-1\right]^2\\ &= \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\,\Gamma(s)\phi(1-s)[\zeta(s)\beta(s)-\zeta(2s)],\\ &\quad c > 1. \end{aligned} \tag{21}$$

In spite of its forbidding aspect, an integral such as the last in Eq. (21) frequently leads quickly to interesting information, either through distorting the contour in some way or transforming it to the real axis. We note in this regard that $\Gamma(s)[\zeta(s)\beta(s)-\zeta(2s)]$ is analytic except for simple poles at $s = 0, 1/2, 1$. As a realistic special case, we consider $F(u) = e^{-au}/u$, for which $\phi(s) = a^s/s$. Although the series converges rapidly enough for large a, it diverges for $a = 0$, and it may be important to evaluate it when a is very small. From Eq. (21), we have

$$S = \frac{a}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\, a^{-s}(1-s)^{-1}\Gamma(s)[\zeta(s)\beta(s)-\zeta(2s)]. \tag{22}$$

Analysis shows that while the integral converges along a large semicircle in the left hand plane for $0 < a < 1$, its value is not vanishingly small along this path. However, its value does go to zero with a. Thus, for small a, the value of S is dominated by the behavior of the integrand at the aforementioned poles ($s = 1$ is now a second order pole), and we obtain

$$S = (\pi/2)\ \ln[\Gamma(3/4)/\Gamma(1/4)(2\pi a)^{1/2}] - (\pi\gamma/4) - 2(\pi a)^{1/2} + o(a), \quad (23)$$

where γ is Euler's constant. This expression is quite accurate for $a \lesssim 0.01$. There is another approach to these sums, which while not having been fruitful in this investigation, is quite suggestive and may be useful in other cases. We write

$$\theta_3^2(0\,|\,t) = \sum_{m,n=-\infty}^{\infty} \exp[(m^2 + n^2)\pi i t] = \sum_n r_2(n) e^{n\pi i t^+},$$

where $t^+ = t + i0$. Hence, by inverting the Fourier series, we obtain

$$r_2(n) = \int_0^2 dt\, \theta_3^2(0\,|\,t) e^{-n\pi i t^+},$$

where $r_2(n)$ is the number of ways of writing n as the sum of two squares. We now have

$$\sum_{m,n} F(m^2 + n^2) = \int_0^2 dt\, \theta_3^2(0\,|\,t)\phi(t^+),$$

where $\phi(t)$ is the Fourier series $\sum_n F(n)e^{-n\pi i t}$. This procedure is closely related to the 'circle method' introduced by Hardy and Ramanujan into analytic number theory.

The identities in Eq. (12) are only three of forty-seven such results listed by Jacobi,[9] and this list itself can be extended indefinitely by considering successively higher derivatives of the Fourier series for the elliptic functions. It thus appears that we have merely scratched the surface and that there remains a wealth of other lattice summations possible by means of the above method. We seem to have exhausted all the simple two dimensional cases and, since the elliptic integral K is related to products of an even number of theta functions, this procedure will furnish results directly only for even dimensional (cubic) lattices. One particularly simple higher dimensional example is

$$\sum_{k_1,k_2,k_3,k_4} (k_1^2 + k_2^2 + k_3^2 + k_4^2)^{-s} = 2^{-2s}(1 - 2^{-s}) \times (1 - 2^{1-s})\zeta(s)\zeta(s-1) \quad (s > 2), \quad (24)$$

which follows from the ninth entry of Jacobi's list. It would appear that there is no bridge to the important three-dimensional case, but the resourceful Jacobi has provided one through the identity[12]

$$\theta_1'(0\,|\,t) = \theta_2(0\,|\,t)\theta_3(0\,|\,t)\theta_4(0\,|\,t). \quad (25)$$

From this it follows that

$$\sum_{l,p,q} (-1)^{p/2}[l^2 + p^2 + q^2]^{-s} = \sum_{l,k} (l^2 + 4k^2)^{-s} + \frac{1}{4}[(1 - 2^{-2s})\zeta(2s) - \beta(2s-1)]. \quad (26)$$

Unfortunately, to evaluate the sum on the right-hand side of Eq. (26) would require a 'q-series,' such as Eq. (12), for the quantity $\pi(kk')^{1/2}K/2$, which is not known, or equivalently, a Landen transformation connecting θ_2 and θ_4, which does not appear to exist. However, Eq. (26) is a new and interesting relation; by the use of identities related to Eq. (25), it should be possible to reduce a number of three dimensional sums and perhaps adduce useful relations among them.

In this paper we have exploited the fact that the Jacobian theta functions provide an analytic procedure for treating number-theoretic problems relating to even sums of squares. However, the sum in (2) is nothing more than the Dirichlet series

$$S = \sum_{n=1}^{\infty} r_2(n) n^{-s} \quad (27)$$

and all that has been accomplished in the way of 'exact' results is to express certain series of this type in terms of the 'simpler' Dirichlet series $\zeta(s)$ and $\beta(s)$. This can also be done by purely number-theoretic means and indeed for a wide class of quadratic forms $Am^2 + Bmn + Cn^2$. Except for the cases considered here, the reductions involve new functions similar to $\zeta(s)$. This will be described in a sequel where purely number theoretic methods will be applied to 'evaluate' the sums in (26).

ACKNOWLEDGMENTS

The author wishes to thank Dr. Edmund Drauglis for suggesting this problem and Dr. R. P. Kenan for stimulating discussions and for programming the calculation for Table II.

APPENDIX

In the series (3) for $\beta(s)$, which converges for $\mathrm{Re}\, s > 0$, the negative terms correspond to integers congruent to 3, and the positive terms to integers congruent to 1

TABLE II.

s	$\beta(s)$	s	$\beta(s)$
0.50	0.667 69	1.00	0.785 40
0.52	0.673 29	1.02	0.789 23
0.54	0.678 81	1.04	0.792 99
0.56	0.684 25	1.06	0.796 70
0.58	0.689 60	1.08	0.800 34
0.60	0.694 89	1.10	0.803 93
0.62	0.700 09	1.12	0.807 46
0.64	0.705 22	1.14	0.810 94
0.66	0.710 27	1.16	0.814 35
0.68	0.715 26	1.18	0.817 71
0.70	0.720 16	1.20	0.821 02
0.72	0.724 99	1.22	0.824 27
0.74	0.729 75	1.24	0.827 47
0.76	0.734 44	1.26	0.830 62
0.78	0.739 06	1.28	0.833 71
0.80	0.743 61	1.30	0.836 75
0.82	0.748 09	1.32	0.839 74
0.84	0.752 50	1.34	0.842 68
0.86	0.756 84	1.36	0.845 58
0.88	0.761 11	1.38	0.848 42
0.90	0.765 32	1.40	0.851 22
0.92	0.769 46	1.42	0.853 97
0.94	0.773 54	1.44	0.856 67
0.96	0.777 55	1.46	0.859 32
0.98	0.781 51	1.48	0.861 94
		1.50	0.864 50

modulo 4. Also, $r_2(n)$, the number of ways n can be represented as the sum of two squares, is just the number of divisors of n congruent to 1 minus the number congruent to 3. Since S_1, e.g., is simply the Dirichlet series $\sum_n r_2(n)/n^s$, the fact that $\beta(s)$ occurs prominently in our considerations is not surprising. By Euler's procedure, we find that

$$\beta(s) = \prod_p (1 - p^{-s})^{-1} \prod_{p'} (1 + p'^{-s})^{-1}, \tag{A1}$$

where $p \equiv 1, p' \equiv 3 \pmod 4$, in analogy to Euler's product for the zeta function. Although such Dirichlet series were studied intensively between 1850 and 1940, a search of the literature has not revealed a detailed discussion of $\beta(s)$, so we present a number of useful results here.

Since the product (A1) converges absolutely for $\mathrm{Re}\, s > 1$, $\beta(s)$ is analytic in this region and has no zeros there. By using (5), we obtain the representation

$$2\Gamma(s)\beta(s) = \int_0^\infty dt\, t^{s-1} \operatorname{sech} t = 2^{1-s}\Gamma(s)\Phi(-1, s, \tfrac{1}{2}), \quad \mathrm{Re}\, s > 0, \tag{A2}$$

which extends the region of analyticity to the entire right half s-plane. It is not difficult to derive the contour integral representation

$$\beta(s) = -\frac{\Gamma(1-s)}{4\pi i} \int_\infty^{(0+)} dz (-z)^{s-1} \operatorname{sech} z, \tag{A3}$$

which converges for all values of s. Thus, $\beta(s)$ is an entire function. From (A3) and the definition of the Euler numbers[4] we easily obtain

$$\beta(-n) = \begin{cases} 0, & n \text{ odd} \\ \frac{1}{2}E_n, & n \text{ even}, \end{cases} \quad n = 0, 1, 2, \cdots, \tag{A4}$$

as well as

$$\beta(2n+1) = [(\pi/2)^{2n+1}/2(2n!)]\,|E_{2n}|, \quad n = 0, 1, \cdots, \tag{A5}$$

$$\beta(2n) = \frac{(-1)^n \pi^{2n}}{4(2n-1)!} \int_0^1 E_{2n-1}(x) \sec \pi x\, dx, \quad n = 1, 2, \cdots.$$

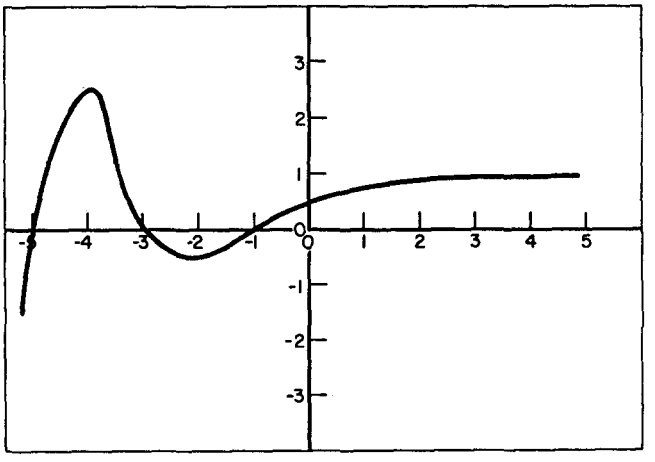

FIG. 1. Qualitative behavior of $\beta(s)$ for real s. For large negative s $\beta(s)$ oscillates with unbounded amplitude.

In particular,

$$\beta(0) = \tfrac{1}{2}, \quad \beta(-2) = -\tfrac{1}{2}, \quad \beta(-4) = \tfrac{5}{2},$$
$$\beta(-1) = \beta(-3) = \cdots = 0, \tag{A6}$$
$$\beta(1) = \pi/4, \beta(3) = \pi^3/32, \ \beta(2) \equiv G = 0.915\ 96\cdots.$$

As for the Riemann zeta function, we have the reflection formula

$$\beta(s) = (\pi/2)^{s-1} \cos(\pi s/2)\Gamma(1-s)\beta(1-s)$$

or

$$2^s\Gamma(s)\sin(\pi s/2)\beta(s) = \pi^s\beta(1-s). \tag{A7}$$

Several values of $\beta(s)$ in the interval $(1/2, \frac{3}{2})$ are given in Table II. From the Hurwitz formula for the generalized zeta function[13] we find

$$\beta(s) = \zeta(1-s, \tfrac{1}{4})\,[(2\pi)^s/2\Gamma(s)\sin(\pi s/2)] + \cot(\pi s/2) \times [(1 - 2^{1-s})/2^s]\zeta(s). \tag{A8}$$

From (A8) we obtain the asymptotic estimates, as $\mathrm{Im}\, s \to \infty$,

$$|\beta(\sigma + it)| \sim \begin{cases} O(|t|^{1/2-\sigma}), & \sigma < 0, \\ O(|t|^{3/2-2\sigma}), & 0 < \sigma < \frac{1}{2}, \\ O(|t|^{1-\sigma}), & \frac{1}{2} < \sigma < 1, \\ O(|t|^{1-2\sigma}), & \sigma > 1. \end{cases} \tag{A9}$$

It is occasionally useful to consider the generalization, for $a > 0$,

$$\beta(s, a) = \sum_{n=0}^\infty \frac{(-1)^n}{[(2n+1)+a]^s}. \tag{A10}$$

By using the analogue of Plana's theorem

$$\sum_{n=0}^\infty (-1)^n \phi(2n+1) = \tfrac{1}{2}\int_0^\infty \mathrm{Re}\,\phi(iu)\operatorname{sech}(\pi u/2)\,du, \tag{A11}$$

we obtain the analogue of Hermite's representation[13] for $\zeta(a, s)$

$$\beta(s, a) = \tfrac{1}{2}\int_0^\infty (a^2 + u^2)^{-s/2} \operatorname{sech}\left(\frac{\pi u}{2}\right) \times \cos\left[s \arctan\left(\frac{u}{a}\right)\right] du, \tag{A12}$$

which converges for all s. Hence, we have the useful representation

$$\beta(s) = \tfrac{1}{2}\left(\frac{2}{\pi}\right)^{1/s} \cos\left(\frac{\pi s}{2}\right) \int_0^\infty du\, u^{-s} \operatorname{sech} u, \quad \mathrm{Re}\, s < 0 \tag{A13}$$

and the results

$$\beta(0, a) = \tfrac{1}{2},$$
$$\left\{\frac{d}{ds}\beta(s, a)\right\}_{s=0} = -2 \ln\left[2\Gamma\left(\frac{a+3}{4}\right)\Big/\Gamma\left(\frac{a+1}{4}\right)\right],$$
$$\beta'(0) = -2 \ln[2\Gamma(\tfrac{3}{4})/\Gamma(\tfrac{1}{4})]. \tag{A14}$$

By use of the reflection formulas, $\beta'(s)$ can be calculated for all integers s. The behavior of $\beta(s)$ for real s is sketched in Fig. 1.

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On the relaxation to quantum-statistical equilibrium of the Wigner–Weisskopf atom in a one-dimensional radiation field. IV. Exact solution for finite systems

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(Received 5 November 1971)

A full study, both analytic and numerical, is made of an exact solution, given in a previous paper of the series, for the problem of the spontaneous emission of a Wigner–Weisskopf atom in a one-dimensional radiation field, when the system is considered to be finite in extent. The solution is obtained directly from the Schrödinger equation of the problem. The numerical solution and results are compared extensively with two separate weak-coupling approximations, treated earlier in the series, which were derived respectively from the Prigogine–Résibois master equation and from the solution of the Schrödinger equation. It is found that the latter corresponds much better, except for exceedingly small systems, with the exact results, and that it accordingly takes better account of the effects due to the nonanalyticity of the solution when the coupling tends to zero. Some proposals are made for the general exploitation in nonequilibrium statistical mechanics of this feature, and also for a possible application to the study of radiationless transitions in molecules.

I. INTRODUCTION

A study has been made in three previous papers of the authors,[1-3] hereafter referred to respectively as I, II, and III, of some problems in the understanding of the Prigogine–Résibois master equation[4] in its weak-coupling form as applied to both finite systems and to systems where the "thermodynamic limit" of finite size has been taken. Attention was directed to the phenomenon of spontaneous emission from the excited state of a two-level Wigner–Weisskopf atom in interaction with a one-dimensional radiation field. It was found that, for the case where the system was enclosed in a finite box (with periodic boundary conditions), the probability of the atom's being excited was a complicated function of time, which manifested Poincaré recurrences on a time scale determined by the length of the box. As the theory was presented in II, this probability was a particular diagonal element of the density matrix of the system. The difficulty arose that its value was not confined to the interval between zero and unity, and it appeared that this was a consequence of a nonanalyticity of the solution of the master equation for the value zero of the coupling constant. This implied, in fact, that, whatever might be the situation for an infinite system, the weak-coupling limit was not well defined in the calculation as performed. The numerical effect of the nonanalyticity, however, was found to be negligible for all but the smallest systems, for which the other reasons could be adduced against any weak-coupling scheme, and so a unique solution to the problem could be found, as far as actual computation was concerned.

An alternative approach was developed in III, where, instead of the master equation for the diagonal elements of the density matrix, the straightforward Schrödinger equation for the state vector of the system was examined. It turned out that a weak-coupling approximation to the solution of this equation existed in the same way as that from the master equation, that is to say, that the probability in question manifested a nonanalyticity for zero coupling which disappeared rigorously in the thermodynamic limit and was unimportant numerically unless the system was very small. But this new approximation shared very few features with the earlier one. Simply from the method of its calculation, it was bounded between zero and one. Its time average had a quite different dependence on the system size from that of the other. The detailed time dependence of the solutions differed widely. About the only similarities, in fact, were, that both gave the same limit for an infinite system and that, for dimensional reasons as much as anything else, the major recurrences appeared at roughly the same times in both.

There seemed to be only one way to decide which, if either, of the weak-coupling approximations for a finite system was a reasonable description of the real evolution, and that was to examine an exact solution to the dynamical problem. This solution was obtained formally in III, both for finite and infinite systems, but it was not analyzed in any detail there. It will be the aim of this paper to perform such a study for finite systems, and it will be seen that a definite choice can be made between the two approximations, at least for all but very small systems.

The mathematical specification of the model has been discussed fully in the previous papers. Briefly, the Hamiltonian describing the two-level atom, the radiation field, and their interaction is:

$$H = H_0 + H_1 = \epsilon_1 \alpha\alpha^* + \epsilon_2 \alpha^*\alpha + \sum_\lambda [\tfrac{1}{2}\hbar\omega_\lambda (a_\lambda^* a_\lambda + 1)] + \sum_\lambda (h_\lambda^* \alpha^* a_\lambda + h_\lambda \alpha a_\lambda^*) \quad (1)$$

in which ϵ_1, ϵ_2 are respectively the energies of the ground state $|1\rangle$ and the excited state $|2\rangle$ of the two-level system. The operators a_λ and α are defined as follows:

$$\alpha = |1\rangle\langle 2|,$$
$$\alpha^* = |2\rangle\langle 1|,$$

$$\langle n_\lambda | a_\lambda | m_\lambda \rangle = [2(n_\lambda + 1)]^{1/2} \delta(m_\lambda - n_\lambda - 1) = \langle m_\lambda | a_\lambda^* | n_\lambda \rangle.$$

The state $|n_\lambda\rangle$ is one with $n_\lambda (= 0, 1, 2, \cdots)$ photons in the λth mode, and $\delta^{kr}(\cdots)$ denotes a Kronecker delta. Following the arguments of I, II, III, we shall choose the coupling h_λ such that

$$|h_\lambda|^2 = \hbar^2 \alpha c^{1-p} E^{1+p} / L |k_\lambda|^p \quad (0 < p < 1) \tag{2}$$

[see Eq. (III-14)] where

$$\hbar E = \epsilon_2 - \epsilon_1,$$

c is the velocity of light, and L is the length of the system. The quantity k_λ, the wavenumber of the λth mode, is given by

$$\omega_\lambda = c |k_\lambda| .$$

In previous work, the radiation field was chosen as one-dimensional, so that one had

$$k_\lambda = 2\pi n / L, \tag{3}$$

with the nonzero integers n labelling the modes, but it will be seen that, for the purposes of this paper, this is not an essential limitation and that one may employ whatever spectrum of values may be suitable for the radiation field with no need to restrict attention to one dimension. Lastly, the dimensionless coupling constant α can be thought of as the fine-structure constant of quantum electrodynamics, or more generally, the parameter which scales the strength of the interaction between the two-level system and the radiation. (For examples of other physical systems with similar Hamiltonians, see Refs. 5 and 6). It should be remarked that the dependence of expression (2) on k_λ was chosen so as to avoid the infrared and ultraviolet divergences of field theory. The states of the system, between which matrix elements of the Hamiltonian, Eq. (1), are to be taken, are given by

$$|i; \{n_\lambda\}\rangle = |i\rangle \prod_\lambda |n_\lambda\rangle$$

with $i = 1, 2$, $n_\lambda = 0, 1, 2, \cdots$. But when the problem of spontaneous emission is considered, that is, when the initial state of the system is taken as

$$|2; \{0\}\rangle, \tag{4}$$

then the only states accessible under the evolution given by H are

$$|2; \{0\}\rangle \quad \text{and} \quad |1; 0, 0, \cdots, 1, 0, 0, \cdots\rangle,$$

where, if the atom is de-excited, there can be only one photon present. These states will be written respectively as $|\mathfrak{A}\rangle$ and $|\lambda\rangle$, where λ ranges over all the modes of the field. If the zero of energy is chosen to be that of the state

$$|1; \{0\}\rangle,$$

—*not* accessible with the initial condition, (4)—then H can be rewritten conveniently as

$$H = \hbar E |\mathfrak{A}\rangle\langle\mathfrak{A}| + \sum_\lambda \hbar\omega_\lambda |\lambda\rangle\langle\lambda| + \sum_\lambda (h_\lambda \sqrt{2} |\lambda\rangle\langle\mathfrak{A}| + h_\lambda^* \sqrt{2} |\mathfrak{A}\rangle\langle\lambda|). \tag{5}$$

In Sec. II, the time-independent Schrödinger equation for the Hamiltonian, Eq. (5), will be solved, and the eigenvalues and eigenkets obtained. From these, the probability of occupation of the state $|\mathfrak{A}\rangle$ at any time will be calculated. This quantity will be examined numerically in Sec. III, and in Sec. IV the numerical results will be compared with those of II and III. Section V contains discussion of the results of the paper and some suggestions for applications and further work.

II. THE EXACT SOLUTION

The eigenvalues Ω and eigenkets $|\Psi\rangle$ of the Hamiltonian, Eq. (5), are obtained from the Schrödinger equation:

$$H|\Psi\rangle = \hbar\Omega|\Psi\rangle. \tag{6}$$

Let us expand $|\Psi\rangle$ in terms of the complete set $|\mathfrak{A}\rangle$, $\{|\lambda\rangle\}$:

$$|\Psi\rangle = c_{\mathfrak{A}} |\mathfrak{A}\rangle + \sum_\lambda c_\lambda |\lambda\rangle.$$

Then Eq. (6) is equivalent to the set of equations:

$$c_{\mathfrak{A}} E + \sum_\lambda c_\lambda (h_\lambda^* \sqrt{2}/\hbar) = c_{\mathfrak{A}} \Omega, \tag{7a}$$

$$c_{\mathfrak{A}} h_\lambda \sqrt{2}/\hbar + c_\lambda \omega_\lambda = c_\lambda \Omega, \tag{7b}$$

whence the secular equation for the eigenvalues Ω:

$$E - \Omega + \sum_\lambda [2|h_\lambda|^2/\hbar^2(\Omega - \omega_\lambda)] = 0. \tag{8}$$

The forms of the Hamiltonian, Eq. (5), and of Eq. (8) show that the problem under consideration is formally identical to a class of problems, the first example of which appears to have been studied by Ullersma,[7] who considered an exactly soluble model for Brownian motion. The scheme of his analysis has been followed by Cukier and Mazur,[8] who examined ergodic properties of an impurity particle in a harmonic chain, and similar methods will be used here. First of all, the nature of the roots of Eq. (8) can be seen from Fig. 1, in which the summation

$$\sum(\Omega) \equiv \sum_\lambda [2|h_\lambda|^2/\hbar^2(\Omega - \omega_\lambda)] \tag{9}$$

is plotted as a function of Ω, along with the linear function $\Omega - E$. It is seen that $\sum(\Omega)$ has poles at the points $\Omega = \omega_\lambda$, that is, at the values of the one-photon energies of each mode of the radiation field. Between these

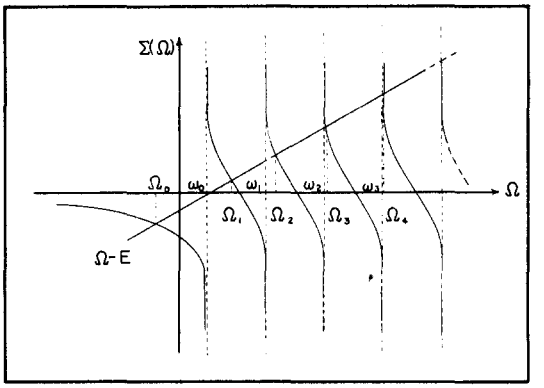

FIG. 1. A plot of $\Sigma(\Omega)$ vs Ω, along with the linear function $\Omega - E$. See the discussion following Eq. (9).

poles, the function $\sum(\Omega)$ has a derivative which is always negative, and so it follows that Eq. (8) has exactly one root in each interval between the successive poles of $\sum(\Omega)$. As $\Omega \to -\infty$, it is clear that $\sum(\Omega) \to 0^-$ as shown in the figure, and that the lowest eigenvalue, Ω_0, is always less than the smallest frequency, ω_0, of the noninteracting field.

To each eigenvalue Ω_i, say, of H, there is a corresponding eigenket, $|\varphi_i\rangle$, say. From Eq. (7), one obtains

$$|\varphi_i\rangle = c^i_{\mathfrak{N}}|\mathfrak{N}\rangle + \sum_\lambda c^i_\lambda |\lambda\rangle,$$

where

$$c^i_\lambda = [h_\lambda\sqrt{2}/\hbar(\Omega_i - \omega_\lambda]c^i_{\mathfrak{N}} \tag{10a}$$

and

$$c^i_{\mathfrak{N}} = (1 + \sum_\lambda [2|h_\lambda|^2/\hbar^2(\Omega_i - \omega_\lambda)^2])^{-1/2} \tag{10b}$$

if $|\varphi_i\rangle$ is normalized so that

$$\langle\varphi_i|\varphi_i\rangle = 1.$$

The choice of the positive square root in Eqs. (10) fixes the phase of $|\varphi_i\rangle$. It is clear that we may write

$$c^i_{\mathfrak{N}} = [1 - \sum'(\Omega_i)]^{-1/2},$$

where the prime denotes differentiation. Now, the system at time $t = 0$ is in the state $|\mathfrak{N}\rangle$, which can be decomposed in terms of the orthonormal eigenkets $|\varphi_i\rangle$ of H:

$$|\mathfrak{N}\rangle = \sum_i [1 - \sum'(\Omega_i)]^{-1/2}|\varphi_i\rangle.$$

Consequently, the probability amplitude for the state $|\mathfrak{N}\rangle$ at time t is:

$$\langle\mathfrak{N}|\Psi(t)\rangle = \sum_i e^{-i\Omega_i t}[1 - \sum'(\Omega_i)]^{-1/2}\langle\mathfrak{N}|\varphi_i\rangle$$
$$= \sum_i \{e^{-i\Omega_i t}/[1 - \sum'(\Omega_i)]\}. \tag{11}$$

This result can readily be seen to be equivalent to Eq. (III-12), which expresses the summation as a contour integral. This formulation proved convenient in the analysis of III, and the result was reached more quickly than here. However, we have preferred to give the present derivation of Eq. (11) in order to point out the similarity of our problem to those of Ullersma, and Cukier and Mazur, as well as to be able to write down the eigenkets of H. Also, for the purposes of the numerical computations of this paper, Eq. (11) gives the solution for the probability amplitude in a more convenient form than that of III.

It is of interest to write down the unitary operator U which diagonalizes the Hamiltonian H:

$$UHU^{-1} = H_D$$

with H_D diagonal in the basis $|\mathfrak{N}\rangle$, $|\lambda\rangle$. We may establish a one-to-one correspondence between the states of this basis and the eigenkets of H as follows: to $|\mathfrak{N}\rangle$ corresponds $|\varphi_0\rangle$, the ket associated with the least eigenvalue Ω_0, and to each $|\lambda\rangle$ corresponds a ket $|\varphi_\lambda\rangle$, say, associated with Ω_λ, the root of Eq. (8) paired with ω_λ in the correspondence seen in Fig. 1. Then U may be written

$$U = |\mathfrak{N}\rangle\langle\varphi_0| + \sum_\lambda |\lambda\rangle\langle\varphi_\lambda|.$$

The unitarity of U follows from the orthonormality of the sets $|\varphi_0\rangle$, $|\varphi_\lambda\rangle$ and $|\mathfrak{N}\rangle$, $|\lambda\rangle$. Its matrix elements are given by

$$\langle\lambda|U|\lambda'\rangle = [h_\lambda\sqrt{2}/\hbar(\Omega_\lambda - \omega_{\lambda'})][1 - \sum'(\Omega_\lambda)]^{-1/2}, \tag{12}$$

and if $|\lambda\rangle$ is replaced by $|\mathfrak{N}\rangle$, Ω_λ is replaced by Ω_0, if $|\lambda'\rangle$ is replaced by $|\mathfrak{N}\rangle$, then the factor

$$h_\lambda\sqrt{2}/\hbar(\Omega_\lambda - \omega_{\lambda'})$$

is replaced by unity.

Lastly in this section, we shall write Eq. (11) in terms of dimensionless variables of the kind employed in I, II, and III. There it was found necessary, in order to give meaning to the notion of weak coupling, to scale times and frequencies by the coupling constant α. Thus, from a time t or a frequency Ω, we define

$$\tau = \alpha E t, \quad \xi = \Omega/\alpha E,$$

where τ and ξ are dimensionless. With the further definition

$$\sigma(\xi) = \sum(\Omega)/\alpha E = \sum(\alpha E\xi)/\alpha E,$$

Eq. (8) becomes

$$\langle\mathfrak{N}|\Psi(\tau)\rangle = \sum_i \{e^{-i\xi_i\tau}/[1 - \sigma'(\xi_i)]\}, \tag{13}$$

where the ξ_i are the roots of the dimensionless secular equation

$$\xi - 1/\alpha - \sigma(\xi) = 0. \tag{14}$$

If now we make use of the definitions (2), (9), then there results

$$\sigma(\xi) = (2/\sigma^2)\sum_\lambda [1/(\alpha\xi_\lambda)^{+p}(\xi - \xi_\lambda)], \tag{15}$$

where

$$\xi_\lambda = \omega_\lambda/\alpha E$$

and the dimensionless scaled length σ^2 is $\alpha EL/c$. If further we now restrict attention to a one-dimensional system with the ω_λ determined by Eq. (3), then Eq. (15) becomes

$$\sigma(\xi) = \frac{4}{\sigma^2}\sum_{n=1}^{\infty} \frac{1}{(2\pi n\alpha/\sigma^2)^p(\xi - 2\pi n/\sigma^2)}, \tag{16}$$

whence also:

$$\sigma'(\xi) = \frac{4}{-\sigma^2}\sum_{n=1}^{\infty} \frac{1}{(2\pi n\alpha/\sigma^2)^p(\xi - 2\pi n/\sigma^2)^2}. \tag{17}$$

These formulas will be useful in the numerical work of the next section.

III. DISCUSSION OF NUMERICAL CALCULATIONS

The first stage of a numerical study of the exact solution given by Eq. (13) was to compute the eigenvalues of the Hamiltonian. This was achieved by considering the equation

$$\xi - \sigma(\xi + 1/\alpha) = 0, \tag{18}$$

whose solutions differ from those of Eq. (14) by $-1/\alpha$. Equation (18) was studied rather than Eq. (14) only to make closer contact with the investigations in III, in which Eq. (III-37) corresponds exactly to Eq. (18) with the approximation:

$$\sigma(\xi + 1/\alpha) = 2\cot(\sigma^2/2)(\xi + \varphi),$$

where φ is the nonanalyticity parameter which, as was discussed in Sec. I, enters the weak-coupling scheme. Here, no attempt was made to use the exact analytic form for $\sigma(\xi + 1/\alpha)$ which is given in III (see Eqs. (III-29, -30, -31). This form is rather complicated, and is far less well suited to computation than the straightforward definition, Eq. (16). Although this remark is made concerning the calculations presented in this paper, which are all restricted to the one-dimensional case with coupling given by Eq. (2), it will be clear from what follows that it can be made general and that there is no great increase in computational difficulty if one considers a different choice of $|h_\lambda|^2$ from Eq. (2), or a different spectrum of frequencies ω_λ, as, for example, in a three-dimensional problem. The quantity $\sigma(\xi + 1/\alpha)$ was calculated, then, from Eq. (16), with α set equal to 0.1, and for two values of σ^2, 1.0 and 10.0. These values of σ^2 are those chosen for the numerical investigations of II and III, and for comparison with those studies it was felt that 0.1 was a suitable coupling, in that it is not so small as to make calculations involving it indistinguishable from those of III, but still it can be considered "weak" coupling. The exponent p was chosen as $\frac{1}{2}$ and $\frac{1}{4}$ for each value of σ^2.

In the numerical work, the eigenvalues, say ξ_i, were determined by a method analogous to the graphical method of Fig. 1, that is, by selecting the points at which ξ and $\sigma(\xi + 1/\alpha)$ were most nearly equal. In the summation, Eq. (16), 10^4 terms were taken, and for $n \geq 10^4$, the remainder was approximated by the integral

$$\frac{2\alpha^{-p}}{\pi} \int_\kappa^\infty \frac{d\kappa}{\kappa^p[\kappa - (\xi + 1/\alpha)]} \quad \text{where} \quad \kappa = \frac{2\pi}{\sigma^2} \cdot n.$$

The error introduced using this procedure is negligible as can be seen from the following example. For the particular choice $\xi = 10.0, \sigma^2 = 10.0, \alpha = 0.1$, and $p = \frac{1}{2}$, the summation (16) gives

$$\sigma(\xi + 1/\alpha) = 2.474\ 5357 \quad \text{for} \quad n = 10^4$$

$$\sigma(\xi + 1/\alpha) = 2.509\ 3190 \quad \text{for} \quad n = 10^5,$$

a difference of 0.034 7833. The difference obtained for this interval using the above integral is 0.034 7844. Since the mesh used in solving Eq. (18) was 0.0001, the slight discrepancy between these two differences is certainly acceptable. Having obtained the eigenvalues ξ_i, we calculated $\sigma(\xi_i)$ using Eq. (17) with the first 100 terms summed exactly, and the contribution to (17) for $n \geq 10^2$ approximated by the integral

$$-\frac{2\alpha^{-p}}{\pi} \int_\kappa^\infty \frac{d\kappa}{\kappa^p[\kappa - (\xi + 1/\alpha)]^2}.$$

From this point, the computation of $\rho(\tau)$, the probability of finding the state $|\mathfrak{N}\rangle$ at time τ, proceeded exactly as in III. There, for $\sigma'(\xi_i)$, the approximation

$$-\sigma^2(1 + \tfrac{1}{4}\xi_i^2)$$

was used, and here, the computed exact values. As there, a separation of $\rho(\tau)$ is made into its time average ρ_c and the purely oscillatory part $\rho_T(\tau)$:

$$\rho(\tau) = |\langle \mathfrak{N}|\Psi(\tau)\rangle|^2 = \left|\sum_i \frac{e^{-i\xi_i\tau}}{1 - \sigma'(\xi_i)}\right|^2 = \sum_i [1 - \sigma'(\xi_i)]^{-2} + \sum_{\xi_i > \xi_{i'}} \frac{2\cos(\xi_i - \xi_{i'})\tau}{[1 - \sigma'(\xi_i)][1 - \sigma'(\xi_{i'})]} = \rho_c + \rho_T(\tau). \tag{19}$$

This expression has obvious analogies with the approximate Eq. (III-36). It has been computed here for 11 roots, ξ_i, for $\sigma^2 = 1.0$ (both for $p = \frac{1}{2}$ and $p = \frac{1}{4}$), and for 100 roots for $\sigma^2 = 10.0$ (for $p = \frac{1}{2}$ and $p = \frac{1}{4}$). In order to assess, the error introduced in the procedure for calculating (17), $\sigma'(\xi_i)$ was determined by summing 1000 terms exactly and then using the integral approximation for $n \geq 10^3$. The value of $\rho(\tau)$ at $\tau = 0$ obtained was then compared with the one obtained using 100 terms in (17). For $\sigma^2 = 10.0, \alpha = 0.1$, and $p = \frac{1}{2}$, the 100-term calculation (with integral correction) gave $\rho(0) = 0.993\ 1982$ while the 1000-term calculation (with integral correction) gave $\rho(0) = 0.993\ 2099$. Similarly, for $\sigma^2 = 1.0, \alpha = 0.1$, and $p = \frac{1}{2}$, the 100-term calculation (with integral correction) gave $\rho(0) = 0.993\ 9357$, whereas the 1000-term calculation (with integral correction) gave $\rho(0) = 0.993\ 9408$. It was the authors' conclusion that the small differences observed did not justify the longer computation time required to perform the 1000-term calculation.

The results of the numerical computations are displayed in Figs. 2–7. The first of these has the results for $\sigma^2 = 1.0$, for p equal to both $\frac{1}{2}$ and $\frac{1}{4}$, and for a range of τ from 0 to 5. The function plotted in each case is $\rho_T(\tau)$, the time-dependent part of the evolution. The values of the constant term ρ_c are given in the caption to the figure. Figure 3 gives the results for $\sigma^2 = 10.0$, this time with a range 0 to 25 of τ. The qualitative aspects of these results are as one would expect: An initial decay over a rather short time scale is followed at later times determined by the size of the parameter σ^2 by large and rapid fluctuations. A convenient characterization of the functions $\rho_T(\tau)$ was developed in III to avoid detailed consideration of their behavior over large ranges of τ. This was to calculate the average fre-

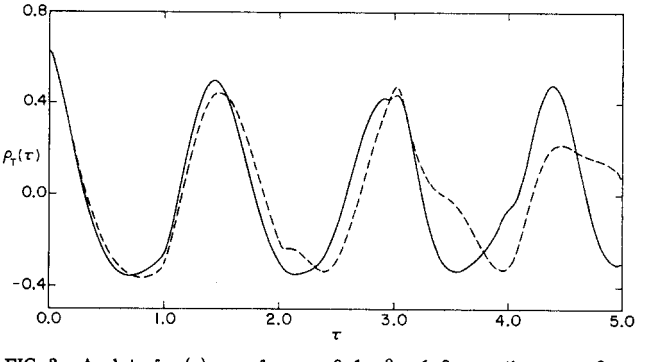

FIG. 2. A plot of $\rho_T(\tau)$ vs τ for $\alpha = 0.1, \sigma^2 = 1.0$ over the range $0 \leq \tau \leq 5$. For the choice $p = \frac{1}{2}$ (solid line), $\rho_c = 0.3659$ and $\rho_T(0) = 0.6281$. For the choice $p = \frac{1}{4}$ (dashed line), $\rho_c = 0.3627$ and $\rho_T(0) = 0.6261$.

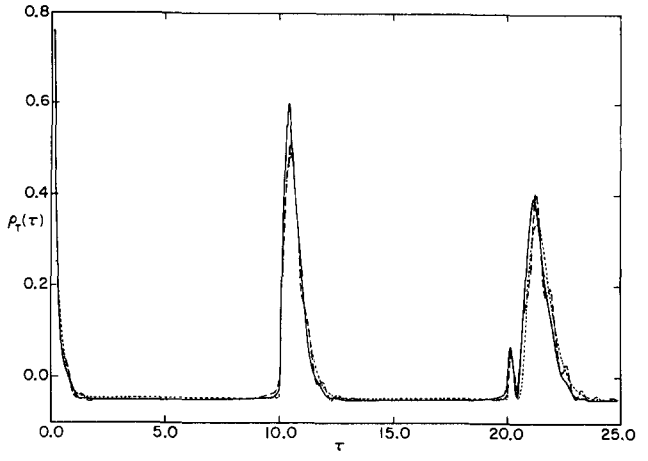

FIG. 3. A plot of $\rho_T(\tau)$ vs τ for $\alpha = 0.1, \sigma^2 = 10.0$ over the range $0 \leq \tau \leq 25$. For the choice $p = \frac{1}{4}$ (solid line), $\rho_c = 0.0497$ and $\rho_T(0) = 0.9360$. For the choice $p = \frac{1}{2}$ (dashed line), $\rho_c = 0.0506$ and $\rho_T(0) = 0.9426$. The dotted line represents the Schrödinger weak-coupling $\rho_T(\tau)$ vs τ for $\sigma^2 = 10.0, \alpha = 0.1$ and phase $\varphi = 0.0$; here, $\rho_c = 0.0465$ and $\rho_T(0) = 0.9335$.

quency $L(q)$ with which such a function attains the value q. This quantity $L(q)$, in addition to subsuming most of the relevant information about a given $\rho_T(\tau)$ into a simple form, gives quantitative estimates of Poincaré recurrences, where these are to be understood in the same way as in III, that is, that although the expression in Eq. (19), involving as it does a linearly independent set of frequencies ξ_i, can never exactly regain its initial value of unity, it may approach it arbitrarily closely. The function $L(q)$ then measures the average frequency of such "near-recurrences." For the purpose of obtaining an accurate estimate of $L(q)$ for the functions $\rho_T(\tau)$ plotted in Figs. 2–3, these functions were computed for $\sigma^2 = 10.0$ at intervals of 0.1 of τ over the range $100 \leq \tau \leq 400$, and for $\sigma^2 = 1.0$, at intervals of 0.02 over the range $0 \leq \tau \leq 150$. These intervals and ranges are the same as those used in comparable investigations in III—in the next section explicit comparisons will be made with that work. Values of $L(q)$ vs q were then obtained by direct counting. Figures 4–5 contain the results of this procedure: $L(q)$ is plotted

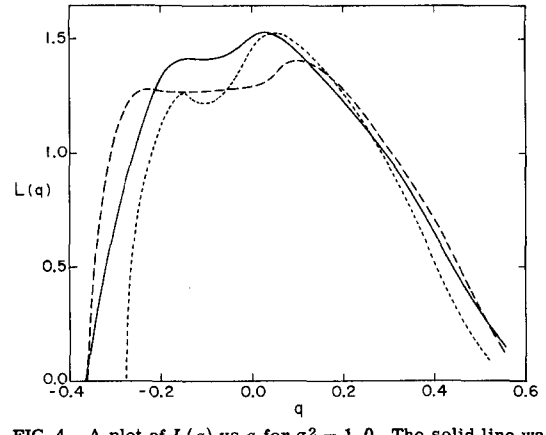

FIG. 4. A plot of $L(q)$ vs q for $\sigma^2 = 1.0$. The solid line was constructed from an analysis of the time-dependent part of $\rho_E(\tau)$ for $p = \frac{1}{2}$, using the counting procedure described in III. A similar analysis was performed for $p = \frac{1}{4}$ (dashed line), and for comparison, the corresponding curve for the weak-coupling Schrödinger solution $\rho_s(\tau)$ (dotted line) is included (for the phase $\varphi = 0, \rho_c = 0.2784$ and $\rho_T(0) = 0.7074$). In constructing these curves for this choice of σ^2, a range of τ $0 \leq \tau \leq 150$ was used.

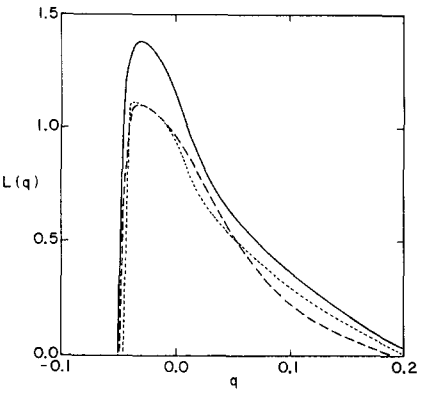

FIG. 5. A plot of $L(q)$ vs q for $\sigma^2 = 10.0$. The solid line was constructed from an analysis of the time-dependent part of $\rho_E(\tau)$ for $p = \frac{1}{2}$. The dashed line refers to a similar analysis for $p = \frac{1}{4}$, and for comparison the curve corresponding to the weak-coupling Schrödinger $\rho_s(\tau)$ solution (phase $\varphi = 0$) is included (dotted line). For this choice of σ^2, a range of τ $100 \leq \tau \leq 400$ was used.

in Fig. 4 for $\sigma^2 = 1.0, p = \frac{1}{2}, \frac{1}{4}$ and in Fig. 5 for $\sigma^2 = 10.0, p = \frac{1}{2}, \frac{1}{4}$. It should be remarked that the sensitive values of q occur about 300 times over the ranges of τ used to obtain these plots, and, from consideration of the scatter about the mean of the number of occurrences in subranges, one may expect a maximum error of about 6% in any value $L(q)$. It would appear then that the appearance of maxima of $L(q)$, or at least a definite flattening of the profile, for $\sigma^2 = 1.0$ is a real effect, and in fact, such a phenomenon was observed in the weak-coupling solution in III.

IV. COMPARISON WITH THE WEAK-COUPLING SOLUTIONS

One of the main objects of this paper is to determine, by comparing them against the exact solution, which, if either, of the weak-coupling approximations to $\rho(\tau)$ discussed in II and III yields a fair description of the real behavior of the system. For the purposes of reference we shall rewrite these approximations here. That which was based on the master equation is [see Eq. (II-40)]:

$$\rho_L(\tau) = \left(1 + \frac{2\sigma \sinh 2\sigma}{\cosh 2\sigma - \epsilon}\right)^{-1} + \sum_{\Theta_p > 0} \frac{2\Theta_p^2}{\Theta_p^2 + 4/\sigma^2} \times \cos\left[\tau\left(\Theta_p^2 + \frac{4}{\sigma^2}\right)^{1/2}\right]\left[1 + \frac{\sigma^2\epsilon}{(1-\epsilon^2)^{1/2}} \times \left(\Theta_p^2 + \frac{16}{(1-\epsilon^2)}\right)^{1/2} + \frac{\sigma^2}{4}\left(\Theta_p^2 + \frac{16}{(1-\epsilon^2)}\right)\right]^{-1}, \tag{20}$$

where Θ_n are the successive positive roots of the equation

$$4 \sin(\sigma^2\Theta) = \Theta L\epsilon - \cos(\sigma^2\Theta)]$$

and where ϵ is a nonanalyticity parameter, equal to $\cos(\sigma^2/\alpha)$. The other approximation, based on the solution of the Schrödinger equation [see Eq. (III-36)] is

$$\rho_s(\tau) = \sum_{\xi_q}[1 + \sigma^2(1 + \tfrac{1}{4}\xi_q^2)]^{-2} + \sum_{\xi_q > \xi_{q'}} \frac{2\cos(\xi_q - \xi_{q'})\tau}{[1 + \sigma^2(1 + \tfrac{1}{4}\xi_q^2)]\cdot[1 + \sigma^2(1 + \tfrac{1}{4}\xi_{q'}^2)]}, \tag{21}$$

where ξ_q are the roots of the equation

$$\xi - 2 \cot \frac{\sigma^2}{2}(\xi + \varphi) = 0$$

with φ a nonanalyticity parameter, equal to

$$1/\alpha - 2 \cot p\pi.$$

These expressions, Eqs. (20) and (21), have to be compared with the exact solution, $\rho_E(\tau)$, say, as given by Eq. (19).

Some remarks must be made about the choices of the coupling function $|h_\lambda|^2$ used in the derivations of Eqs. (19), (20), and (21). In this paper, as in the derivation leading to Eq. (21), it was given by Eq. (2), but in II, where Eq. (20) was derived, it was given by

$$|h_\lambda|^2 = \hbar^2 \alpha c E/L, \tag{22}$$

which corresponds to Eq. (2) with $p = 0$. This latter choice gives rise to divergences in the theory developed in III, but not in that of II. It was, however, a conclusion of III that for σ^2 large enough—and in particular $\sigma^2 = 10.0$ is large enough—$\rho_s(\tau)$ is essentially independent of the nonanalyticity parameter φ. But it is only through φ that the exponent p enters Eq. (21), and so we may claim that this solution is to hold for any choice of p in Eq. (2), even for $p = 0$. Similar consideration may be adduced for Eq. (20), where again there will be practically no dependence of $\rho_L(\tau)$ on p if Eq. (2) is used for $|h_\lambda|^2$ rather than Eq. (22), provided only that σ^2 is large enough. We shall conclude, then, that with this proviso Eqs. (20) and (21) are directly comparable, and comparable also with Eq. (19) for any choice of p. This conclusion is not by any means a startling one, since one knows that in the *weak-coupling limit*, all these equations lead to the same exponential decay in the thermodynamic limit:

$$\rho_\infty(\tau) = e^{-4\tau} \tag{23}$$

[see Eqs. (II-32) and (III-23)], a result dependent only on the value of $|h_\lambda|^2$ for $\omega_\lambda = E$. So long, then, as α is small enough that there is a weak-coupling situation, we may reasonably expect that even the exact solution, Eq. (19), will be insensitive to the value of p for all but small σ^2. But precisely this has been seen in the last section, where, even for $\sigma^2 = 1.0$, the characterizations $L(q)$ for the two values of p were found to differ by very little.

In Fig. 6, the three solutions, ρ_L, ρ_s, and ρ_E, have been plotted on the same graph for $\sigma^2 = 1.0$ and a time range $0 \leq \tau \leq 5$. The plots of ρ_L and ρ_s have been taken respectively from Fig. 7 of II and Fig. 3 of III, with the choices of the nonanalyticity parameters used there, namely $\epsilon = -0.84$ and $\varphi = 0.0$. For ρ_E, p was taken as $\frac{1}{2}$. It is immediately evident that the three curves are all quite different, apart from the broadest general aspects. It has been remarked in the preceding section, however, that, for $\sigma^2 = 1.0$, such differences also exist between two curves of ρ_E, both derived from Eq. (19), but with different values of p (Fig. 2). The same feature was found with ρ_s (see Figs. 3 and 4 of III). More illuminating, then, is Fig. 3, where in addition to the two profiles of ρ_E (for the choices $p = \frac{1}{2}, \frac{1}{4}$) ρ_s has been plotted for $\sigma^2 = 10.0$ and a time range $0 \leq \tau \leq 25$ (see

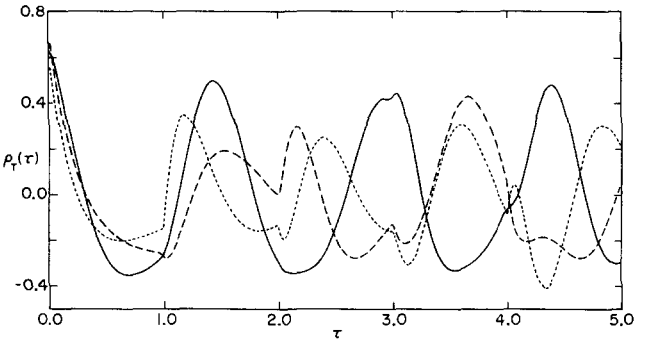

FIG. 6. A comparison of the time-dependent part of $\rho_E(\tau)$ (solid line), $\rho_s(\tau)$ (dashed line), and $\rho_L(\tau)$ (dotted line), for $\sigma^2 = 1.0$ over the range $0 \leq \tau \leq 5$. For $\rho_E(\tau)$, $p = \frac{1}{2}$ and for $\rho_s(\tau)$, $\varphi = 0$.

Fig. 2 of III). Here the similarities in the three profiles are much more marked than their differences. This is to be noted in conjunction with the results of the last section and of III, where it was seen that dependence of ρ_s on φ and of ρ_E on p had ceased to be observable on the plots for $\sigma^2 = 10.0$. The curve of ρ_L, on the other hand, has been omitted from this figure, since it is known from III (see also Fig. 8 of II) that it differs markedly from that of ρ_s and hence also from ρ_E.

The next useful comparison that can be made is of the functions $L(q)$ associated with the quantities ρ_s and ρ_E. Again, ρ_L will be omitted from this study, since it has already been seen in III that the profile of $L(q)$ vs q is rather different in structure from the one corresponding to ρ_s; in particular, for ρ_L the profile was symmetric, whereas for ρ_s, the profile was definitely skew. For $\sigma^2 = 1.0$, it has been seen (see Fig. 6 of III) that the dependence of $L_S(q)$ on φ is slight (in fact, considering the margin of error involved in the determination of the function, the two curves are essentially identical). From Fig. 4, one sees that the dependence of $L_E(q)$ on p for this value of σ^2 is somewhat more pronounced, but over all, an examination of this figure with its plots of $L_E(q)$ (for $p = \frac{1}{2}, \frac{1}{4}$)and $L_S(q)$ (for $\varphi = 0$) reveals that all three profiles are remarkably similar. Similar plots of $L_E(q)$ and $L_s(q)$ vs q are given in Fig. 5, where the same result, as one might expect, is found.

Finally, in this section, it has been thought worthwhile to exhibit a direct comparison of ρ_s and ρ_E, with $\sigma^2 = 10.0, \varphi = 0, p = \frac{1}{2}, \frac{1}{4}$ for some large values of τ. This has been done in Fig. 7, for the range $100.0 \leq \tau \leq 125$. The resemblance between the three profiles, in the authors' opinion, is striking if one considers the nature of Eqs. (19) and (21), with their summations of many terms involving cosines, even small discrepancies in the arguments of which might be expected, because of the large values of τ, to lead to very considerable effects in the time-dependencies of ρ_s and ρ_E. It should be remarked that the correspondence between the profiles ρ_s and ρ_E for $p = \frac{1}{2}$ is preserved even up to the longest times considered in this study, that is, $\tau = 400$. The resemblance is less evident for ρ_E with $p = \frac{1}{4}$ for values of τ greater than around 200, but it is possible that this effect is due to inaccuracies in the numerical computation of ρ_E with $p = \frac{1}{4}$, for which value calculations of Eqs. (16) and (17) are perhaps less reliable than for $p = \frac{1}{2}$. On the other hand, the results in Fig. 7 are an agreeable confirmation of the validity of the numerical methods which gave rise to them.

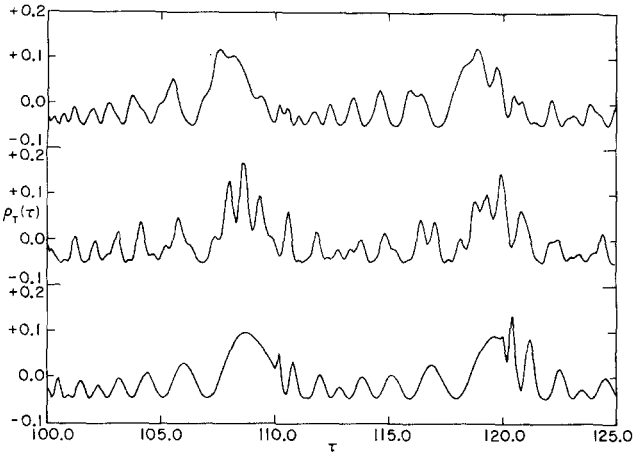

FIG. 7. A comparison of $\rho_E(\tau)$ for two choices of $p, p = \frac{1}{4}$ (upper curve) and $p = \frac{1}{2}$ (middle curve), and $\rho_s(\tau)$ for a phase $\varphi = 0$ (lower curve), for $\sigma^2 = 10.0, \alpha = 0.1$ over the range $100 \leq \tau \leq 125$.

V. DISCUSSION AND CONCLUSIONS

The principal conclusion of this paper is clearly that, for the description of the spontaneous emission of the Wigner–Weisskopf atom in a finite box with weak coupling, the approximate method used in III and based on the quantum-mechanical solution derived from the Schrödinger equation is much better than the method of II, which came from consideration of the lowest-order terms in the master equation. There are probably several reasons that this should be so. Firstly, all the ideas that lead to the master-equation approach to nonequilibrium phenomena are rooted in the notion of a *large* system, as well as that of weak coupling, and there is no reason to suppose *a priori* that such an approach will give good results for small systems. The equations of quantum mechanics, on the other hand, are explicitly constructed to deal with small systems. Thus, although in the thermodynamic limit the weak-coupling solution of the master equation is the correct one, this solution is not reached as the limit of an equally correct description of a finite system. It must be noted therefore that attempts at a rigorous justification of the master equation for infinite systems should *not* proceed from its predictions for finite systems, which are not valid, but rather from the true dynamics of these systems as given, presumably, by quantum mechanics. The whole concept of a weak-coupling approximation, of course, breaks down for very small systems (for example, $\sigma^2 = 1.0$) where the nonanalyticity in the coupling parameter that is always present away from the thermodynamic limit becomes an important effect. This means that it cannot be claimed even for the approach of III, based on the Schrödinger equation, that it yields a proper approximation for the case of small systems. But, as is quite evident from the calculations performed for $\sigma^2 = 10.0$, it does indeed provide a very good approximation once the effects of nonanalyticity cease to be important. So much so in fact, that it is probably possible to devise a still simpler approximation that would preserve the main qualitative features of the exact result.

The second remark to be made in favor of the solution ρ_s over ρ_L is that ρ_s, as given in Eq. (21), is obtained directly as an approximation to the *exact* solution, Eq. (11), by taking an approximate estimation of $\sigma(\xi)$. This is in contrast to ρ_L, which is the solution, in the weak-coupling limit, of an equation, namely the master equation in lowest order, that is already only an approximation. Now, exact solutions are seldom available for problems of physical interest, and it is the function of the master equation to provide a perfectly definite prescription under certain conditions—large size, weak coupling—for treating systems for which no exact result can be obtained. Such generality cannot at this stage be claimed for the method employed in III. It has recently been shown by Pike and Swain[9] that another technique used with much success in statistical mechanics, both of equilibrium and nonequilibrium, that of double-time Green's functions, leads for our model to precisely the same result for $\rho(\tau)$ as does the master equation, namely ρ_L. We would like to suggest that, in view of this and of the well-known difficulties in finding rigorous validations of any of the methods of nonequilibrium statistical mechanics, the good agreement which has been found between ρ_s and ρ_E is a strong argument for investigating further the possibility of developing systematic approximate treatments which would lead to results like those of III and would permit thermodynamic solutions to appear as the limit of approximations for finite systems whose closeness to the exact solutions of quantum-mechanical equations of motion could be demonstrated.

There exists a hope that the model studied in this paper of a finite system, along with either its exact solution, Eq. (19), or the good approximation, Eq. (21), might, over and above the suggestion of the preceding paragraph, be of explicit use in an attempt to understand the phenomenon of radiationless transitions[10] in certain medium-sized molecules. These transitions are characterized by the transfer of the energy of some—more or less isolated—excited electronic state to a set of closely-spaced levels of similar energy associated with a different configuration of the molecule. This process occurs in several molecules, which may be classified according to the density of the levels to which relaxation takes place. Different effects are observed depending on whether the levels are sparse or rather so close as to form a quasicontinuum. These differences may well be related to the differences found in our model between small systems, with a sparse density of photon states, and larger systems, with a higher density.

Finally, to return to the question of the thermodynamic limit, we may point out that the exact solution of this paper allows a discussion of a system, in this limit, with arbitrary coupling. The simple exponential behavior, Eq. (23), which results from no matter what approach for a large system, is of course valid for weak coupling only. In I certain problems have been considered which arise because the corrections to Eq. (23) needed if the coupling is not small seem to be, like all the solutions examined in this paper, nonanalytic in α, and to be in consequence nonexponential. Such behavior can be expected in the thermodynamic limit of the exact solution also, and comparisons can thus be made between the nonexponential contributions to it and those predicted by the master equation when taken beyond lowest order. The analysis of these matters is the subject of the next paper in this series (immediately following), and it may be regarded as the first step towards the understanding of the relationship for an infinite system between the master equation and the exact limit of the solution of the equations of motion for a finite system.

ACKNOWLEDGMENTS

One of us (R.D.) thanks the F.R.F.C. of Belgium for financial support while this work was being performed. The other (J.J.K.) has benefited from funds provided to the University of Notre Dame by the National Science Foundation. This work was supported in part by the United States Atomic Energy Commission through contract AT(11-1)-38.

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